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# Operation of the Institute for Computer Applications in Science and Engineering

Final Report for NASA Grant NGR 47-102-001

Covering the Period

July 1972 - September 1975

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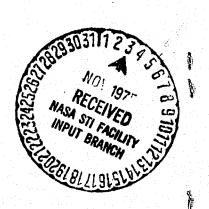
IN SCIENCE AND ENGINEERING

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This document and the attached reports constitute the final report of NASA Grant NGR 47-102-001 awarded to the Universities Space Research Association, a consortium of some fifty major universities across the country in 1972 to operate the Institute for Computer Applications in Science and Engineering (ICASE) at NASA's Langley Research Center.

The primary objective of ICASE is to perform research in applied mathematics, numerical analysis, and applied computer science with particular emphasis on application areas of interest to the Langley Research Center. The mechanism of performing such research is through visiting appointments of leading university researchers in these fields, postdoctoral fellowships, and term appointments of younger scientists with no other affiliation. Such appointees, whose training is primarily in mathematics and computer science, are encouraged to work in close collaboration with NASA scientists and engineers on problems of mutual interest. It is hoped that such collaborations will contribute to the continued vitality of applied mathematics and computer science while at the same time make either immediate or long term impact on problems of concern to NASA.

The overall research program of ICASE is directed toward the general area of scientific computing with particular emphasis on bridging the many gaps between theory and practice, and between mathematicians or computer scientists on the one hand and engineers or natural scientists on the other. The major categories of the ICASE research program are:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR-100.
- b. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.

- c. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.
- d. Computer systems and software, with particular emphasis on minicomputers, data management, and computer graphics.

In the following paragraphs research activities in these categories are enumerated; more detail may be found in the semi-annual reports that we attached. This research effort has produced 39 technical papers which were either submitted to journals for publication or presented at national conferences for which there were proceedings. In addition, the research has benefited from an active seminar program that has included a total of 136 talks.

Throughout the period of the grant a total of ten people have worked solely or in part on vector and parallel computers. This effort produced eight technical papers. Seven of the talks in the ICASE seminar program dealt with the subject.

The research on vector and parallel computers has been divided between numerical analysis for linear algebra and non-numeric computer science.

Below is a list of topics that have produced or are expected to produce technical papers. In addition an annotated bibliography of over 200 entries was compiled.

# Linear Algebra

- . Comparison of techniques for solving tridiagonal systems on the STAR-100.
- . Analysis of algorithms for banded and dense linear systems for the STAR-100.
- Analysis of the dissection algorithms for solving the linear system arising from finite element approximations on a general vector computer.
- . Solution of recurrence relations on parallel computers.

- . Analysis of the block cyclic reduction algorithm.
- . Consideration of the Lanczos and conjugate gradient algorithms for vector computers.

#### Non-numeric

- . A study of the STAR-100 operating system with particular emphasis on the impact of virtual memory.
- . Support of a project to develop a new vector language for the STAR-100.
- . Analysis of algorithms for sorting on a vector computer.
- A study of the possible imbalance in the time required to solve a banded linear system too large to reside in main memory versus the time to move the system from secondary storage into main memory.

A total of twenty people have worked solely or in part in the area of numerical analysis during the period of the grant. Thirteen technical papers resulted from this effort. The ICASE seminar program included sixty-one talks in this area.

The research in numerical analysis has been divided among linear algebra, approximation theory and differential equations. Below is a list of topics that have produced or are expected to produce technical papers.

#### Linear Algebra

- . Development and comparison of algorithms for the reduction of the bandwidth and profile of large sparse matrices.
- . The minimization of ||Ax-b|| in the uniform norm.
- The investigation of solving sparse matrix problems by considering companion sparse matrices which are close to the original but easier to solve.
- . Analysis of the Lanczos and conjugate gradient methods for large sparse systems.

Development of an algorithm for obtaining some or all of the interior eigenvalues and associated eigenvectors of a large sparse matrix.

#### Approximation Theory

- . Development of an algorithm for least squares approximation with linear inequality constraints.
- Construction of a package of computer routines for performing approximation using splines under tension.
- . Investigation of the secant method for nonlinear least squares problems.

#### Differential Equations

- . Study of techniques for the numerical integration of stiff ordinary differential equations in real time.
- The application of successive overrelaxation to elliptic boundary value problems where the relaxation factor is permitted to vary over the region.
- . Generalization and analysis of the DuFort-Frankel scheme for parabolic partial differential equations.
- . Study of the well-posedness of the compressible Navier-Stokes equations with constant total temperature.
- . Analysis of the stability of spectral methods for initial-boundary value problems for hyperbolic equations.
- . Generalization and study of the Lax Wendroff and Leap-Frog schemes for hyperbolic equations.

In addition to the above research, packages of computer programs were made operational for linear programming and a fast Poisson solver. ICASE also served as a test site for EISPAK, a package of programs for eigenvalue problems.

Throughout the period of the grant a total of twenty-three people have worked solely or in part on computational research in engineering and the natural sciences. This effort produced eleven technical papers. Twenty-four of the ICASE seminars were in this area.

The research has been divided among fluid flow, structural dynamics, acoustics, and computational chemistry. The topics listed below have produced or are expected to produce technical papers.

#### Fluid Flow

- . Simulation of ocean circulation by the finite element method.
- . Study of three dimensional flow in a square inlet,
- . Study of boundary conditions that can be imposed on the outflow region.
- . The analysis of flow about axisymmetric blunt bodies at hypersonic speeds.
- . Initialization of the equations of dynamic meteorology.
- . Development of an alternating direction iterative method particularly well suited for the nonlinear parabolic equations or the Navier Stokes equations.
- . Development of a model of turbulence based on the spectral distribution of the turbulent energy.
- . Application of the Multi-Level Adaptive Technique to transonic flow.
- . A comparison of the efficiency of various methods for solving the Navier Stokes equations.
- . Study of the appropriate boundary conditions for the base of a hypersonic reentry body.

### Structural Dynamics

. The finite element method applied to two-dimensional elasticity and beam problems.

- . The study of the motions of a clamped plate excited by supersonically convected turbulence.
- . The investigation of nonlinear waves in elastic plates.

#### Acoustics

- . The study of the propagation of sound through a realistic subsonic jet flow field.
- . The modeling of a turbulent subsonic jet.

#### Computational Chemistry

- The solution of the Schrodinger equation to investigate the oxidation of atmospheric constituents.
- . Calculation of the bond energy and entropy of the complex HaNHC1.

A total of thirteen people have worked solely or in part on computer systems and software during the period of the grant. Seven technical papers have resulted from this research. A total of forty-four of the ICASE seminars dealt with computer systems and software.

The research has been divided among computer systems, grahics, data base management and software engineering. Much of this work was made possible by the presence of computer hardware acquired under NASA supplemental grant NSG 1072.

#### Computer Systems

- . Development of a trace driven computer simulation of the Langley Research Center computer system to investigate job scheduling.
- The installation of a PRIME 300 minicomputer system and the implementation of various software improvements on that system.

#### Graphics

- . Installation of the National Center for Atmospheric Research graphics package on the Langley and ICASE computer systems.
- . Study of the feasibility of using a minicomputer for interactive graphics.
- Design and construction of a microcomputer system for enhancing the graphics capability of the extremix 4014 terminal.

### Data Base Management

- . Investigation of data base management systems based on set theory.
- . Study of buffer management in data base systems.
- . Evaluation of the data management requirements of an integrated aircraft design program.

#### Software Engineering

- . Study of the role of structured programming in software development.
- . Investigation into the prevention, detection, and classification of software errors.

In addition to the above formal research program, ICASE sponsored several other activities. Four short courses of approximately one week each were conducted. The topics were Advanced Linear Algebra, Stability Theory for Difference Approximations to Time Dependent Partial Differential Equations, Theory and Application of Singular Values, and Computer Graphics. Approximately fifty people attended each of these courses.

ICASE has also been involved in sponsoring technical meetings. The first of these was the summer meeting of the Society for Industrial and Applied Mathematics in 1973. It was attended by over 400 people from universities, industry and government. In the fall of 1974, a meeting on numerical analysis

for parallel and vector computers was attended by over 200 people. ICASE was a joint sponsor with the NASA Langley Research Center of a conference on the application of computer graphics in engineering in the fall of 1975. This meeting attracted over 250 people.

There are five ICASE reports included as part of this final report.

The first of these is an annual report for the period September 1, 1972 
August 31, 1973. The remaining four are semi-annual reports covering the period September 1, 1973 - August 31, 1975. These reports will provide more detail on the research that was itemized above.

# INSTITUTE FOR COMPUTER APPLICATIONS IN

SCIENCE AND ENGINEERING (ICASE)

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ANNUAL REPORT

September 1, 1972 - August 31, 1973

#### 1. Introduction

ICASE was formed in July of 1972 under an agreement between the NASA Langley Research Center and the Universities Space Research Association (USRA). Dr. A. R. Kuhlthau, President of USRA, served as Acting Director of ICASE from July, 1972 to November, 1972. During this period an executive assistant, Mr. John C. Tredennick, and a secretary, Mrs. Myrtle Wells, were hired and established an ICASE office in Bldg. 1220. In addition, an advisory committee, consisting of Dr. John J. Donovan of the Massachusetts Institute of Technology, Dr. James M. Ortega of the University of Maryland, and Dr. Robert H. Owens of the University of Virginia, met several times with Dr. Kuhlthau to establish goals and directions for ICASE. Subsequently, Dr. Ortega was offered and accepted the position of Director and served in this capacity on a part-time basis from December, 1972 to May, 1973, at which time he assumed the duties full time. In March of 1973, Dr. Robert G. Voigt was selected as Assistant Director.

The ICASE research program began in earnest in May, 1973, and consists of four major categories:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR-100.
- b. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
- c. Analysis and planning of large-scale software systems.
- d. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.

The work in each of these areas will be described in detail in the next section. Other activities are discussed in Section 3 while Section 4 gives a prognosis of the next year's activities.

Prior to May, 1973, the major activities of the ICASE staff were (a) establishing administrative practices for the organization, (b) planning the research programs, (c) publicizing ICASE and recruiting a staff, (d) preparing for the First Langley Conference on Scientific Computing, and (3) sponsoring a lecture series.

#### 2. The ICASE Research Program

#### a. Efficient Use of Vector and Parallel Computers

Since his appointment in March, 1973, Dr. Voigt has taken responsibility for this area and has devoted most of his time, apart from administrative duties, to becoming familiar with the CDC STAR and with the literature on parallel and vector processing, for which he is currently compiling a bibliography. Dr. Voigt is now working, partly in conjunction with members of the Analysis and Computation Division (ACD), on developing algorithms for the STAR for the numerical solution of matrix problems, with emphasis on the solutions of systems of linear equations.

John C. Knight, Assistant Professor of Computer Science at West Virginia University, spent the period May 14 to August 11, 1973, at ICASE working on certain aspects of the hardware and software of the CDC STAR. This work was done in cooperation with ACD and, in particular, Mr. Everett Johnson. The hardware design of the STAR was examined in order to provide detailed understanding of its operation and to detect

possible areas of deficiency and inefficiency. The investigation of the software was limited to the central resource allocation aspects of the operating system. CDC's proposals were examined and possible shortcomings discussed. Alternative algorithms based on the "working set" theory were proposed, and a considerable effort was made to incorporate results which have been published in the computer science literature into the design of the algorithms. Rather little detail has been given in the above description since Prof. Knight's investigations have been published in an ICASE report.

Alan Feldstein, Associate Professor of Mathematics at Arizona State University, was at ICASE for the period July 30 - August 25, 1973. He continued work being done in conjunction with Professor Joe Traub of Carnegie-Mellon University on the problem of solving nonlinear systems of equations on parallel computers. The current work on this project is being directed towards the case of a single equation in a single unknown. Results are being obtained as to rate of convergence of different algorithms as a function of the number of processors. Prof. Feldstein presented his work at an ICASE colloquium.

# b. Numerical Analysis

The work in numerical analysis, independent of that reported above in connection with vector processors, consisted of mainly consulting activities by short-term visitors.

Jorge More, Assistant Professor of Computer Science at Cornell University, spent the period July 2 - July 13, 1973, at ICASE. Prof. More gave a colloquium talk and consulted with several Langley staff members about problems of mutual interest. In particular, he exchanged some programs and reports with Terry A. Straeter of ACD, discussed some nonlinear problems in finite element structure analysis with Ahmed K. Noor of George Washington University, assisted Ernest S. Armstrong of the Flight Dynamics and Control Division in disproving a conjecture on a problem in control theory, and discussed possible solution techniques for singular linear systems with Susan Voigt of the Structures Division.

Prof. Sven-Ake Gustafson, of the University of Stockholm (Sweden), spent the period July 23, 1973 - August 10, 1973, at ICASE working in close cooperation with ACD to implement and document a numerically stable FORTRAN code for linear programing. Most linear programing routines are based on the algorithms by Charnes and Dantzig. However, these are generally numerically unstable and often break down yielding infeasible solutions or otherwise useless results. A possible remedy would be to reinvert the basis at each iteration but this proves costly if the number of variables and constraints is large. Instead of updating the inverse of the basis one can update its LU or QR decomposition in a stable and economical manner. Algol codes employing LU decompositions have been published but no FORTRAN codes could be secured. To translate the Algol codes into FORTRAN was deemed a very difficult task and instead a decision was made to develop new codes from scratch following an account of the theory (Bartels, R. H.,

Golub, G. H., and Saunders, M.A.: Numerical Techniques in Mathematical Programing in Nonlinear Programing, ed. Rosen, Mangasarian, and Ritter, Academic Press (1970)). The resulting code is capable of solving unstructured linear programs using stable updating of the LU form. The computing time per iteration is proportional to m<sup>2</sup> where m is the dimension of the basis. The code can be expected to be a useful tool for the solution of discretized versions of problems in approximation, convex and semi-infinite programing, and is now available from ACD.

James W. Daniel, Associate Professor of Computer Science and Mathematics at the University of Texas, Austin, spent the week August 13 - August 17, 1973, at ICASE. Prof. Daniel also gave a colloquium lecture and participated in several discussions with Langley personnel. These included an informal second lecture on some problems in optimal control, discussions with Terry A. Straeter of ACD on air traffic control and other problems in optimization, discussions with John N. Shoosmith of ACD on two-point boundary value problems, a meeting with John E. Hogge and others from ACD on spline approximation, and discussions with some members of the Structures Division on various optimization problems.

Dr. Jerrold S. Rosenbaum will begin a one-year appointment at ICASE on September 1, 1973, and spent several days at ICASE during July and August. During this period, he discussed the problem of numerical integration of ordinary differential equations with Roland L. Bowles of ACD with the expectation of working in cooperation with Bowles in the future.

#### c. Software Systems

Stephen W. Sherman, Assistant Professor of Computer Science at the University of Houston, spent the period May 21 to August 31, 1973, at ICASE. His primary activity has been to produce a trace-driven computer simulation model of the ICOP's operating system which links the five 6000 computers together at Langley. The purpose of this work is to investigate various algorithms for job scheduling. The number of variables involved in job scheduling and the number of possible scheduling algorithms are both very large, and for the present problem analytical models were not feasible. Likewise, implementation of different scheduling algorithms on the actual operating system is impractical. This dictated some kind of computer simulation model and trace-driven modeling, in which a recorded trace of system activities is directly used to define the environment and workload, was considered to be the best solution. The model would not only allow investigation of job scheduling, but could also be used for predicting the effects of changes in configuration, printing algorithms, tape mounting algorithms, and various other modifications. The model is now in the final stages of implementation with programing support furnished by ACD, and an ICASE paper describing this model, its implementation, and preliminary results obtained by the model is in preparation. The program will be turned over to ACD personnel who will continue to use this tool for further investigations of improvements in ICOPS.

In the course of the above work, Prof. Sherman has also considered various ways in which the performance of ICOPS could be improved. In particular, in another ICASE paper, he discusses in

some detail the concept of "swapping" and how it might be used to enhance job scheduling as well as various other functions such as tape mounting.

# d. <u>Computational Research in Engineering and Science</u>

Dr. Stanely F. Birch spent the period March 8 April 6, 1973, at ICASE working in conjunction with Dennis Bushnell of
the Hypersonic Vehicles Division compiling information on present and
future computational and theoretical methods in turbulence modeling.
This work has been reported in an ICASE publication.

George J. Fix, Associate Professor of Computer Science and Applied Mathematics at the University of Maryland and now Associate Professor of Mathematics at the University of Michigan, spent the period May 21- August 24, 1973, at ICASE. During this period, Prof. Fix's efforts were devoted primarily to the development of finite element approximations to the Navier-Stokes equations with attention to higher order quadratic and cubic elements. There were two basic applications of this work. The first was to ocean circulation problems. This material, along with a theoretical analysis, was presented at the SIAM National Meeting in June and is summarized in an ICASE publication, which will be submitted to the SIAM Journal on Applied Mathematics. Since the work is available in report form no further details will be given here. The second application was to a two-dimensional flow problem. This work, which used a cubic element developed by Prof. Fix, was done in conjunction with Dennis Bushnell and Charles Cooke of the Hypersonic Vehicles Division. An ICASE publication, jointly authored by Cooke and Fix, is in preparation and will describe this project in detail.

In addition, Prof. Fix consulted with various other members of the Langley staff on problems in finite element approximations and fluid dynamics.

Yi-Yuan Yu, Distinguished Professor of Aerospace Engineering at Wichita State University, spent the period May 21 - August 21, 1973, at ICASE, working on finite element approximations for certain structures problems.

Ever since the finite element method in structural analysis was recognized as being a generalization of the Rayleigh-Ritz method, variational principles have become a powerful tool for its further advancement. More recently, the use of Galerkin's method in finite element formulation has attracted attention. The method is important because its use does not depend on the existence of a variational principle. On the other hand, its proper use is at times difficult to determine and it is useful to look into the situation in the light of the variational equation, assuming that a variational principle does exist.

Two linear problems have been examined. One is that of two-dimensional elasticity, and the other that of a classical beam. Some difficulties arise when the finite element formulation is carried out on the basis of Galerkin's equations. Through the use of the variational equation, however, these difficulties are explained and resolved.

In addition to providing a solid basis for finite element formulation, the variational equation is also a potentially powerful tool for solving nonlinear problems. This is demonstrated by considering a third problem of vibrations of beams with large deflection. The great

flexibility that can be achieved through the use of the variational equation in the solution of a problem in general and in the finite element formulation in particular is clearly indicated.

Of particular interest in the problem of nonlinear vibrations of beams is to study the dependence of the frequency on the vibration amplitude. To solve the nonlinear algebraic equations an iterative numerical procedure was proposed and with assistance from the Analysis and Computations Division a computer program was prepared and some numerical results are being obtained. A report on this work is in preparation by Professor Yu.

Stanley G. Rubin, Associate Professor of Aerospace Engineering at Brooklyn Polytechnic Institute spent the period June 25 - August 24, 1973, at ICASE. He was joined during most of this period by two of his students, Mr. Michael C. Distefano and Mr. Frank J. Tarulli, who received nominal subsistence support from ICASE. Prof. Rubin, together with his students, carried on three projects in computational fluid dynamics during this period. The first concerned incompressible transient jet motion. The transient behavior of fluids injected into an unbounded quiescent ambient or into a finite chamber is being considered. These flows appear in combustion chambers, in multiple jet interactions, and in sewage disposal. The two-dimensional unbounded case will serve as a test on the applicability of the numerical formulation. The stream function-vorticity system will be evaluated by overrelaxation and iterative predictor-corrector methods, respectively.

In order to optimize the numerical procedure and still retain all the essential features of the fluid mechanics a coordinate transformation reflecting the Navier-Stokes behavior near the orifice and boundary layer characteristics for downstream has been formulated.

This transformation incorporates the appropriate algebraic decay far from the central core of the injected fluid and the exponential decay near the jet boundaries.

Preliminary results have led to several important modifications on the treatment of the surface and far-field boundary conditions. Further analysis of the flow behavior in these regions will be required before detailed calculations are feasible. This work will eventually be published as a thesis by Mr. Distefano.

The second project dealt with supersonic flow at the leeplane of a cone at incidence. There have been numerous studies concerned with the flow over cones at incidence. For moderate angles of attack, most of these analyses have failed to adequately describe the leeplane behavior. It has been conjectured that the boundary layer similarity approximation is the reason for this failure. Detailed calculations, for the similarity model, have been made in order to resolve the leeplane anomaly. An implicit marching technique has been applied in order to evaluate the boundary layer behavior. Initial conditions at the windward plane were obtained with an iterative method for two-point boundary value problems. A complete non-similar solution has previously been determined. It is shown that although the similarity method converges at all points arbitrarily close to the leeplane, significant errors occur at locations three to five degrees from the leeplane, where mass is entrained in the outer portions of the boundary layer at a rate in

excess of that allowable with the similarity assumption. This work will comprise a M.S. thesis for Mr. Tarulli.

The third project concerned three-dimensional flow in a square inlet. The boundary layers that form along the walls of an inlet induce crossflows and streamwise pressure gradients. Analytic treatment of the entrance region suggests a swirling crossflow pattern previously undetected by numerical analysis. As the boundary layers grow they fill the channel and the analytic model must be reexamined in order to determine the evolution of the boundary layer induced crossflow patterns.

Alternating-direction-implicit and overrelaxation iterative methods are used in order to evaluate the streamwise velocity and vorticity, and crossflow behavior, respectively. Compatibility requires a complex iteration procedure in order to insure mass continuity and the proper convection of vorticity. The appropriate iteration scheme is currently under investigation and it is evident from preliminary results that the crossflow behavior is extremely sensitive to the iteration procedure. The streamwise velocity is relatively insensitive and therefore does not provide a good measure for the accuracy of the numerical method.

# 3. Other ICASE Activities

Since October, 1972, ICASE has sponsored a colloquium lecture series. These lectures have been held at least monthly and sometimes more often; a complete list of the speakers and the titles of their lecture is given in appendix A. All of these speakers participated in discussions with Langley staff during their visit and a few (e.g. Prof. Stone and Dr. Concus) stayed over for an additional day or two of

consultations.

On June 18-21, 1973, at the Sheraton Conference Center in Hampton, ICASE cosponsored, with the Society of Industrial and Applied Mathematics (SIAM) and the Special Interest Group on Numerical Mathematics of the Association of Computing Machinery, the First Langley Conference on Scientific Computing. This conference was held in conjunction with the 1973 SIAM National Meeting, for which ICASE was the official host. (Dr. Ortega served as General Chairman for the meeting and co-chairman of the Program Committee, Dr. Voigt served as Chairman for Contributed Papers, and Mr. Tredennick served as Chairman of Local Arrangements.) The conference consisted of a symposium on Symbolic Mathematical Computation, with five invited talks, and a second symposium on Computational Problems in Partial Differential Equations with eight invited talks. The speakers for these 13 talks are listed in Appendix B. In addition, there were approximately 100 contributed 15 minute papers on various topics in applied mathematics presented at the SIAM meeting, and Mr. Edgar M. Cortright, Director of NASA Langley Research Center, was the Luncheon Speaker on June 20. Approximately 350 people attended the conference and all reports indicate that the meeting was considered successful.

Another activity of ICASE was concerned with the three local graduate programs in computer science. On July 13 and again on August 20 representatives of George Washington University, Old Dominion University, and the College of William and Mary met at ICASE to discuss further cooperation and communication between the programs.

Some concrete outcomes of these meetings were: (a) the cross-listing of two courses between ODU and W and M during the Fall Semester, 1973.

(b) a comparison and discussion of the tentative schedules in computer science of the three institutions for the Spring Semester, 1974, with the purpose of possibly deleting overlaps, filling gaps, and cross-listing of other courses as appropriate.

It was agreed to continue monthly meetings of the group and to explore additional ways of cooperation between the three programs including the possiblity of closed circuit TV between the various locations.

#### 4. A Prognosis for the Next Year

In this section we will outline, as much as is possible at the present time, the program of ICASE during the year September 1, 1973 - August 31, 1974. We will use the same major research categories as in Section 2.

# a. Efficient Use of Vector and Parallel Computers

The ICASE personnel primarily involved in this area will be Dr. Voigt, Dr. William Poole, Assistant Professor of Mathematics at the College of William and Mary who is spending the 1973-74 academic year at ICASE, and Dr. Alan Cline of the National Center on Atmospheric Research, who will join ICASE in September on a one-year appointment. It is planned that these three will collaborate with three or four people from ACD to form a "working group" on mathematical subroutines for the STAR. This group will begin work early in September with its first goal to analyze possible algorithms for basic linear algebra problems (solution of systems of linear equations, etc.) and make

recommendations for subroutine implementation. This will build on the work already done by ACD's STAR Project Office. It is hoped that the group will be able to move on to other areas, such as partial differential equations, as rapidly as possible. Dr. John Shoosmith of ACD and Dr. Ortega will participate in the group's activities as much as possible.

Prof. John Knight will remain in contact with ICASE and ACD during the coming academic year and plans to be at Langley for two weeks during the Christmas vacation. He will return to ICASE for the summer of 1974 to continue his work on scheduling algorithms and other aspects of the software of the STAR.

It is anticipated that various other members of ICASE.will become involved with the STAR in due course.

# b. Numerical Analysis

Dr. Jerrold Rosenbaum will conduct research in the numerical solution of ordinary differential equations, especially so-called stiff equations. Part of this work will likely be done in connection with the simulation computations at Langley and preliminary discussions with Roland Bowles of ACD have already begun. It is quite possible that this will lead to consideration of the STAR in the near future.

Dr. Rosenbaum will also teach a graduate course in his specialty at William and Mary College during the 1973 Fall Semester.

A. Kadir Aziz, Professor of Mathematics at the University of Maryland will spend the academic year September 1, 1973 - June 1, 1974, at ICASE while on sabattical leave. He will work primarily on the theory of finite element methods as applied to hyperbolic partial

differential equations, but is also very interested in doing collaborative work with Langley personnel on applied problems.

Karen R. Credeur will commence a one-year appointment at ICASE early in Fall, 1973, when she completes her Ph.D. requirements in Statistics at Harvard University. She has several possible problems under consideration but, in any case, will likely spend a portion of her time developing computational methods in statistics.

Gene H. Golub, Professor of Computer Science at Stanford University, will spend the week of September 6-12 at ICASE. Prof. Golub is one of the world's leading experts on computational matrix problems and it is anticipated that several people at ICASE, ACD, and other areas of Langley will benefit from his advice.

Alan George, Assistant Professor of Computer Science at the University of Waterloo, will spend December 3-14, 1973, at ICASE consulting on problems dealing with finite element methods, numerical solution of large sparse system of equations, and other problems.

Drs. Cline, Poole, and Voigt are also likely to contribute to the general area of numerical analysis in the course of their investigations on algorithms for STAR.

One or two additional appointments, especially in the area of numerical solution of partial differential equations, are anticipated in the next year.

# c. <u>Software Systems</u>

On September 24-25, 1973, ICASE will host a meeting of three of the leading experts in the country on operating systems, for

the purpose of discussing present and future trends of computer systems in general and to make recommendations to ACD on the future development of the computer complex at Langley. The three are Prof. James Browne, Chairman of Computer Science at the University of Texas at Austin, Dr. R. Stockton Gaines of the Institute for Defense Analysis in Princeton, and Prof. Saul Rosen of Purdue University. They will be joined by Prof. Steve Sherman of the University of Houston, who spent the summer of 1973 at ICASE and was instrumental in initiating this endeavor. (It is hoped, incidentally, that Prof. Sherman will return to ICASE for the summer of 1974 to continue the work reported in Section 2.)

Dr. W. Terry Hardgrave, currently a research associate at CERN, will join ICASE on January 1, 1974, on a one-year appointment. Dr. Hardgrave's main interests are in data management techniques and operating systems and it is expected that he will collaborate with the Structures Division on data management problems in the IPAD system as well as with ACD on questions concerning the operating system.

It is hoped that ICASE will be able to add another person in operating systems and someone in interactive computer graphics during the next year.

d. Computational Research in Engineering and Science

Virginia Jordan, currently Assistant Professor of
Mathematics at William and Mary College, will join ICASE on September 1,
1973. This will initially be a part-time appointment while she finishes
the requirements for her Ph.D. in Applied Mathematics at Harvard University. The portion of her ICASE supported time will be devoted to
work in collaboration with Charles Whitlock of the Space Applications

and Technology Division on a problem involving the effect of winds on waves off the Atlantic coast. This will involve theoretical investigation as well as computational work at the appropriate time.

Dr. Max Gunzburger, currently a Post-doctoral Fellow at the Naval Ordinance Laboratory, will commence a one-year appointment at ICASE in September, 1973. Dr. Gunzburger's specialty is mathematical fluid dynamics and he will work primarily in collaboration with the Acoustics Branch of the Loads Division on problems of mutual interest. He will also devote a portion of his time to basic research in the numerical solution of partial differential equations.

Dr. David Yen, Professor of Mathematics and of Material Science at Michigan State University, will spend the period January 1 - June 30, 1974, at ICASE while on sabbatical leave. He plans to continue his research on nonlinear waves in elastic beams and plates as well as interact strongly with Langley staff on problems in acoustics and fluid dynamics.

Dr. Richard C. Raffenetti, currently a Post-doctoral Fellow at Batelle Memorial Institute, will join ICASE early in 1974 on a one-year appointment. He will work primarily with Dr. Donald Phillips of the Environmental and Space Sciences Division on problems in computational physical chemistry. He also plans to become involved with the STAR at an early date.

In addition to the above research areas, ICASE plans to continue its colloquium lecture series through a combination of invited speakers as well as ICASE members in residence. We are also looking

shead to sponsoring the Second Langley Conference on Scientific Computing, probably in the Fall of 1974. The theme of this conference would likely be "vector and parallel processing." Discussions with Ames Research Center have begun on possible joint sponsorship, due to their interest in the Illiac IV computer.

# Appendix A.- Colloquium Lectures

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October 30, 1972	Prof. Cleve B. Moler, University of New Mexico; The NATS Project for Mathematical Subroutines
December 11, 1972	Prof. C. William Gear, University of Illinois; Automatic Solution of Ordinary Differential Equations
January 22, 1973	Prof. Steven A. Orszag, Massachusetts Institute of Technology; Turbulence and Compulence
February 26, 1973	Prof. William Kahan, University of California, Berkeley; How to Help An Ill-Posed Problem Get Well
March 26, 1973	Prof. Carl de Boor, University of Wisconsin; The Representation of Piecewise Polynominal Functions in A Computer; B-Splines
May 7, 1973	Prof. G. W. Strang, Massachusetts Institute of Technology; Illegal Finite Elements and the Patch Test
May 11, 1973	Dr. Rodney R. Oldehoeft, Purdue University; Design of NAPSS-Like Systems
May 14, 1973	Prof. Harold S. Stone, Stanford University; Perfect Shuffle Algorithms
May 23, 1973	Prof. George J. Fix, University of Maryland; Finite Element Methods for Fluid Flow
June 4, 1973	Dr. Patrick J. Roache, Sandia Laboratories; Finite-Difference Methods for the Steady-State Navier-Stokes Equations
June 8, 1973	Dr. Myron Lecar, Smithsonian Institution; On the Original Distribution of the Asteroids
June 13, 1973	Dr. Paul Concus, Lawrence Berkeley Laboratory; Iterative Use of Fast Direct Methods for Elliptic Equations
June 15, 1973	Dr. James R. Miller, National Center for Atmospheric Research; Computational Analysis of Stratified Free Shear Flows
July 2, 1973	Prof. Jorge J. More, Cornell University; Quasi-Newton Methods

# Appendix A. Colloquium Lectures

August 3, 1973 Prof. Alan Feldstein, Arizona State University; Root Finding on Parallel Computers

August 13, 1973 Prof. James W. Daniel, University of Texas
A Conjugate Gradient Approach to Nonlinear
Elliptic Boundary Value Problems Over
Irregular Regions

# Appendix B. Invited Lectures at the First Langley Conference on Scientific Computing

June 18, 1973	Dr. Richard Jenks, IBM, Symbolic Mathematical Systems; The State of the Art
June 18, 1973	Prof. John D. Lipson, University of Toronto; Algebraic Algorithms: Theory and Practice
June 19, 1973	Prof. Anthony C. Hearn, University of Utah; Problem Solving by Symbolic Computation
June 19, 1973	Prof. Joel Moses, Massachusetts Institute of Technology; The Exponential Case of the Risch Integration
June 19, 1973	Prof. William M. Kahan, University of California, Berkeley; One Numerical Analyst's Experience with One Symbol Manipulator
June 20, 1973	Prof. Cleve B. Moler, University of New Mexico; A New Look at Some Old Methods for Partial Differential Equations
June 20, 1973	Prof. Jim Douglas, Jr., University of Chicago; The Location of Points at which Finite Element Solutions are Very Accurate
June 20, 1973	Prof. Gene H. Golub, Stanford University; Direct Methods for Elliptic Difference Equations
June 20, 1973	Prof. Paul R. Garabedian, New York University; Survey of Some Recent Research in Transonics
June 21, 1973	Prof. C. K. Chu, Columbia University; Computational Fluid Dynamics: Survey and Observations
June 21, 1973	Prof. George J. Fix, University of Maryland & ICASE; Numerical Models for Ocean Circulation Problems
June 21, 1973	Prof. Martin H. Schultz, Yale University; A Comparison of Finite Element Methods
June 21, 1973	Prof. J. A. George, University of Waterloo; Sparse Matrix Techniques in the Direct Solution of Finite Element Equations

#### Appendix C.- Reports and Publications

- 1. Birch, Stanley F.: A Review of Numerical Problems Associated with Turbulence Modeling. ICASE, July 18, 1973.
- 2. Knight, John C.: Scheduling Central Resources on the C.D.C. STAR 100. ICASE, August 29, 1973.
- 3. Fix, George J.: Finite Element Approximation of Ocean Circulation Problems. ICASE, August 27, 1973.
- 4. Sherman, Stephen W.: Suggestions of Operating System and Software Improvements for ICOPS. (In preparation)
- 5. Sherman, Stephen W.: A Trace-Driven Model of the Integrated Computer Operating System at NASA Langley Research Center. (In preparation)
- 6. Cooke, Charlie H., and Fix, George J.: A Finite Element Solution Algorithm for the Two-Dimensional Compressible Navier-Stokes Equations. (In preparation)

# Appendix D. - ICASE Personnel

#### I. Permanent Staff

James M. Ortega, Director Ph.D., Mathematics, Stanford University, 1962 Numerical Analysis

Robert G. Voigt, Assistant Director Ph.D., Mathematics, University of Maryland, 1969 Numerical Analysis

John C. Tredennick, Executive Assistant

Myrtle H. Wells, Secretary

# II. Visiting Staff (January 1, 1973 - September 1, 1973)

- Stanley F. Birch Ph.D., Engineering Science, Dartmouth College, 1971. Fluid dynamics. At XCASE from March 8 to April 8, 1973.
- John C. Knight Ph.D., Computer Science, University of Newcastle-upon-Tyne, Fall 1973 (expected). Assistant Professor of Computer Science at the University of West Virginia. Virtual and paged memories, especially for the STAR. At ICASE from May 14 to August 15, 1973.
- George J. Fix, III Ph.D., Mathematics, Harvard University, 1968. Associate Professor of Applied Mathematics at the University of Maryland. Numerical methods for partial differential equations and, in particular, finite element methods for fluid dynamics. At ICASE from May 21 to August 24, 1973.
- Yi-Yuan Yu Ph.D., Engineering Mechanics, Northwestern University, 1951, Distinguished Professor of Aeronautical Engineering, Wichita State University. Structural analysis. At ICASE from May 21 to August 21, 1973.
- Stephen W. Sherman Ph.D., Computer Science, University of Texas at Austin, 1972. Assistant Professor of Computer Science at the University of Houston. Operating systems. At ICASE from May 25 to August 31, 1973.
- Stanley G. Rubin Ph.D., Aeronautics, Cornell University, 1963.
  Associate Professor of Aerospace Engineering at Brooklyn Polytechnic Institute. Numerical solution of viscous flow problems. At ICASE from July 1 to September 1, 1973, and then at Old Dominion University the rest of the academic year.

### Appendix D.- ICASE Personnel

# II. Visiting Staff (January 1, 1973 - September 1, 1973)

- Jorge J. More Ph.D., Mathematics, University of Maryland, 1970.
  Assistant Professor of Computer Science at Cornell University.
  Numerical analysis and numerical solution of nonlinear equations and optimization problems. At ICASE from July 2 to July 13, 1973.
- Alan Feldstein Ph.D., Mathematics, University of California at Los Angeles, 1965. Professor of Mathematics at Arizona State University. Numerical analysis and parallel algorithms. At ICASE from July 30 to August 24, 1973.
- James W. Daniel Ph.D., Mathematics, Stanford University, 1965.
  Associate Professor of Mathematics & Computer Science, University of Texas at Austin, Mathematical programming and optimization.
  At ICASE from August 13-17, 1973.

# III. Visiting Staff (September 1, 1973 - \_\_\_\_)

- A. Kadir Aziz Ph.D., Mathematics, University of Maryland, 1958. Professor of Mathematics at the University of Maryland at Catonsville. Nonlinear partial differential equations and finite element methods for gas dynamics problems. At ICASE from September 1, 1973, to June 1, 1974.
- William G. Poole, Jr. Ph.D., Computer Science, University of California at Berkeley, 1970. Assistant Professor of Mathematics at the College of William and Mary. Development of algorithms for streaming/pipeline processing. At ICASE from September 1, 1973, to June 1, 1974.
- Jerrold S. Rosenbaum Ph.D., Electrical Engineering and Computer Science, Columbia University, 1971. Numerical solution of ordinary differential equations. At ICASE on one-year appointment.
- Karen R. Credeur Ph.D., Statistics, Harvard University, (expected Fall 1973). Computational statistics and data analysis. At ICASE on part-time basis while completing thesis and then will start one-year appointment.
- Virginia S. Jordan Ph.D., Applied Mathematics, Harvard University, (expected January, 1974). Differential equations and fluid dynamics. At ICASE on part-time basis while completing thesis and then will start one-year appointment.
- Susan M. McCabe B.S., Mathematics, William and Mary College, 1973. Graduate student at William and Mary. Will work half time at ICASE starting September 1, 1973.

### Appendix D. - ICASE Personnel

# III. Visiting Staff (September 1, 1973 -

Gene H. Golub - Ph.D., Mathematics, University of Illinois, 1959. Professor of Computer Science at Stanford University. Largescale matrix problems and numerical solution of partial differential equations. At ICASE September 6-13, 1973.

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- Alan K. Cline Ph.D., Mathematics, University of Michigan, 1970. Senior scientist at NCAR. Computational linear algebra and approximation theory. Will join ICASE on September 23, 1973, on a one-year appointment.
- Max D. Gunzburger Ph.D., Mathematics, New York University, 1969. Fluid dynamics and numerical solution of partial differential equations. Will join ICASE September 17, 1973, on a one-year appointment.
- George J. Fix Ph.D., Mathematics, Harvard University, 1968.
  Associate Professor of Mathematics at the University of Michigan. Numerical methods for partial differential equations and, in particular, finite element methods for fluid dynamics. Will return for short visit in Winter of 1973 and again for Summer of 1974.
- John C. Knight Ph.D., Computer Science, University of Newcastleupon-Tyne, Fall 1973 (expected). Assistant Professor of Computer Science at the University of West Virginia. Virtual and paged memories, especially for the STAR. At ICASE for short visit in Winter, 1973, and then for the Summer of 1974.
- Alan George Ph.D., Computer Science, Stanford University, 1971.
  Assistant Professor of Computer Science, University of Waterloo.
  Numerical linear algebra and finite element methods. At ICASE
  December 3-15, 1973.
- Harold Stone, Associate Professor of Computer Science and Electrical Engineering, Stanford University. Parallel Processing. Short visit in Fall, 1973.
- W. Terry Hardgrave Ph.D., Computer Science, University of Texas at Austin, 1972. Research Associate at Cern. Data management and operating systems. Will join ICASE on January 1, 1974, on one-year appointment.
- Richard C. Raffenetti Ph.D., Physical Chemistry, University of Iowa, 1971. Postdoctoral fellow, Batelle Institute. Computational chemistry. Will join ICASE on January 1, 1974, on one-year appointment.
- David H. Y. Yen Ph.D., Mathematics, New York University, 1965.

  Professor of Mathematics and Metallurgy, Michigan State University.
  Engineering Mechanics. At ICASE January 1 June 30, 1974.

# INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING (ICASE)

Semi-Annual Report

September 1, 1973 - February 28, 1974

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#### 1. Introduction

ICASE was formed in July of 1972 under an agreement between the NASA Langley Research Center and the Universities Space Research Association (USRA), a consortium of over fifty universities across the country. Dr. A. R. Kuhlthau, President of USRA, served as Acting Director of ICASE until November, 1972 when Prof. James M. Ortega of the University of Maryland accepted the position of Director on a part-time basis until May of 1973 and full-time thereafter.

The research program at ICASE began in earnest in May of 1973, and was performed during the summer of 1973 largely by visiting faculty from several universities. These activities were described in the annual report covering the period September 1, 1972 to August 31, 1973.

The research program consists of the following major categories:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR series.
- Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
- c. Analysis and planning of large-scale software systems.
- d. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.

The work in each of these areas will be described briefly in the next section, while other activities are discussed in Section 3.

## 2. The ICASE Research Program

## a. Efficient Use of Vector and Parallel Computers

Dr. Robert G. Voigt, Assistant Director of ICASE, has devoted most of his activity, apart from administrative duties, to this area. He and Mr. J. J. Lambiotte of the Analysis and Computation Division (ACD) are now finishing a joint paper on the best ways to solve tridiagonal systems of equations on vector and parallel computers, and the STAR computer in particular. This problem is a basic subproblem or a prototype for many extensive computations, including the solution of partial differential equations by implicit methods. They, in consultation with Prof. Gene Golub of Stanford University, have analyzed various standard methods for sequential machines as well as some new methods proposed primarily for the Illiac IV and other parallel computers. In addition, they have reformulated the method of cyclic reduction in a form suitable for the STAR. For fairly large N, the dimension of the linear system, this method seems to be the most promising for STAR. For example, based on the latest timing information available, cyclic reduction will be 3 - 4 times faster for N = 1000 than gaussian elimination using scalar code; this ratio increases to about a factor of 7 as N increases. On the other hand, for N less than about 100, it appears that no known method is going to be faster than scalar gaussian elimination. An ICASE report on this work is in preparation.

Professor William G. Poole is spending the year September 1, 1973 - August 31, 1974 at ICASE on leave from William and Mary College. He and Dr. Voigt are in the final stages of completing an annotated bibliography on numerical methods for vector and parallel machines. This will appear shortly as an ICASE report and then be

submitted to Computing Reviews.

Poole and Voigt also are working on a gaussian elimination program for linear equations using an adaptive pivot strategy. The goal is that interchanges, a relatively costly operation on STAR, would not be required nearly as often as with the usual partial pivoting strategy particularly when a solution of only a few digits accuracy is acceptable.

Dr. Alan Cline has been investigating the potential of using Lanczos' method for solving very large sparse linear systems of equations on the STAR. This method seems particularly suited to the STAR vector and sparse vector capability. However, the basic convergence and stability properties of the method are not yet understood on sequential machines and Cline is currently carrying out a mathematical analysis as well as extensive numerical testing on the CDC 6600.

Many of the above activities have been stimulated by, and coordinated with, the work of ACD through a series of meetings of a "STAR Linear Algebra Working Group" consisting of several members of both ICASE and ACD.

A major cooperative effort between the Structures Division, ACD, George Washington University and ICASE has recently begun with the goal of producing a pilot finite element program for the STAR-65 by the summer of 1974. Dr. James M. Ortega of ICASE is assisting Prof. A. Noor of George Washington University in the organization of the work and various ICASE people are cooperating on certain aspects of the problems; Drs. Poole and Cline are assisting in the development of the numerical methods, and Dr. Terry Hardgrave in data management questions. The

group, consisting of about 12 people, has had regular meetings since January 1, 1974 and is now breaking up into subgroups to begin detailed work on the program.

Prof. John C. Knight of West Virginia University spent the summer of 1973 at ICASE working in conjunction with ACD on problems concerning the operating system and virtual memory of the STAR. He returned for the period January 3-11, 1974 to continue this work in anticipation of returning again for the summer of 1974.

## b. Numerical Analysis

In this section, we will review work done in the analysis and development of numerical algorithms with no particular emphasis on the STAR computer. It should be recognized, however, that many times there is no clear dividing line beweeen the two efforts.

Dr. Poole completed a paper, in collaboration with Profs. N. Gibbs and P. Stockmeyer of William and Mary, on band width reduction of large sparse matrices; this work will appear as a joint ICASE and William and Mary report in the near future. Many linear systems of equations which arise in finite element and finite difference methods are sparse (i.e., have many zero elements in the coefficient matrix) and efficient solution of these systems requires utilization of this sparsity. A particularly nice form of sparsity is when the coefficient matrix is banded (i.e., all elements are zero except in a number of diagonals clustered about the main diagonal). In this case, efficient algorithms are available and the amount of work required is proportional to the square of the band width. Hence, various algo-

rithms have been proposed to permute the rows and columns of a sparse matrix in order to reduce the band width before solving the system of equations. Poole, Gibbs, and Stockmeyer have developed a new (heuristic) algorithm for carrying out this band width reduction and have tested it extensively against the Cuthill-McKee algorithm, probably the best one currently available. Their tests have shown that they are usually able to achieve the same or slightly smaller bandwidth in about one quarter of the time required by the Cuthill-McKee algorithm.

Poole also completed a short note on expected pivot size in gaussian elimination. The conclusion, based on certain statistical assumptions, is that the expected pivot size for the partial pivoting strategy is almost as large as for complete pivoting. This work appeared in an ICASE report and was submitted to Mathematics of Computation.

A closely related problem with gaussian elimination is the need for pre-scaling. Drs. Cline and Poole are currently re-examining this question.

A standard computational problem is to find a least squares solution of a linear system of equations Ax = b. Alternately, one could try to find a vector x which minimizes ||Ax - b|| in any other norm and the uniform norm is a natural choice in certain applications. Cline has developed a new method for this problem which obtains the solution after a finite number of trial solutions have been examined in a sequence in which the norm of the residual constantly decreases. The implementation of the method exploits efficient matrix decomposition updating schemes resulting in reduced computation times

when compared with a presently popular method. This work is complete and an ICASE report is in preparation.

Prof. A. Kadir Aziz, on leave for the 1973-74 academic year from the University of Maryland, has been investigating the appliancation of the finite element method to hyperbolic and mixed hyperbolicelliptic partial differential equations. In particular, a major part of this effort has been directed to the study of equations of the form  $g(x,y)\phi_{XX} + \phi_{yy} = f$  where g can change sign in the domain of the problem. Considerable progress has been made both in questions of existence and uniqueness of solutions of the differential equation as well as in the theory of finite element methods as applied to such equations. Work is continuing on this project.

Dr. Jerrold Rosenbaum has been working on new numerical integration schemes for stiff systems of ordinary differential equations, and also adapting known schemes to particular problem classes in order to gain computational efficiency.

One class of new integration schemes is an extension of the generalized trapezoidal rule. For some problems information is known about the time rate of change of the Jacobian and the generalized trapezoidal rule has been extended to make use of this additional information. "Quasilinear" methods based on both quadrature and numerical differentiation have been developed. The methods are now being tested.

Adaption of numerical integration methods to Real Time
Aircraft Simulation is being undertaken by Dr. Rosenbaum in conjunction
with Dr. R. Bowles of ACD. The most promising techniques so far investigated are the generalized trapezoidal rule (developed by Rosenbaum)

and the local linearization method (developed by Bowles, et al). Both methods involve exponential functions of a matrix and further work is being undertaken to find approximations of the exponential function that are particularly suited to the simulation problem.

Atmospheric chemistry equations are another class of problems being investigated in conjunction with Drs. R. Boughner and R. Grose and Mr. R. Graves of the Space Systems Division. The trapezoidal rule was adapted by Dr. Rosenbaum to the problem by using non-standard predictors, and step size controllers. Also, estimators for both local and global errors are being tested. In preparation is a short report on the "mass conservation" properties of numerical integration methods. It is hoped that the "quasi-linear" methods being developed will be applicable to chemistry problems.

In addition, Rosenbaum has consulted with Mr. G. Young of the Space Applications and Technology Division on some problems in two-dimensional quadrature.

Ms. Susan McCabe, a graduate student at William and Mary College, has been providing programming support for much of the research in numerical methods.

# c. Software Systems

Dr. Stephen Sherman, Assistant Professor of Computer Science at the University of Houston, spent the summer of 1973 at ICASE developing a trace-driven simulation model of the current ICOPS operating system at Langley. The purpose and a description of this work is given in the last annual report and, in more detail, in an ICASE report (see Appendix B). During Prof. Sherman's absence during the Fall semester, work on this project has continued under the aegis of ACD and Sherman spent the period

January 7-11, 1974 at ICASE consulting with ACD. The program is now in the final stages of debugging and a second report containing results of the simulation will be prepared in the near future,

Dr. Sherman was also a participant in a two-day meeting at Langley to consult with members of ACD on the current status of the ICOPS operating system and future possibilities of enhancing the system. The other members of this group of consultants were Dr. James Browne, Professor and Chairman of Computer Science at the University of Texas; Dr. Stockton Gaines of The Institute for Defense Analyses; and Dr. Saul Rosen, Professor of Computer Science and Director of the Computation Center at Purdue University, A written report of the recommendations of this group was sent to the Chief of ACD after the meeting.

Dr. W. Terry Hardgrave joined ICASE in early January 1974. His main research interest is in data management systems and he has spent a part of his time since his arrival working with the Structures Division on the data management aspect of the IPAD development. This work has taken two forms. First, he is evaluating the Boeing and General Dynamics feasibility studies with respect to the data base capabilities proposed in these reports. Secondly, he is beginning investigation of two complementary approaches to data management, the first through the use of extended set theory and the second through networking. These two approaches are not exclusive and, moreover, are of general interest in data management systems and not restricted to just the IPAD system. It is expected that this study will continue for the next several months.

# d. Computational Research in Engineering and Science

Prof. George Fix of the University of Michigan and Prof. Charles Cooke of Old Dominion University continued work on a problem begun in the summer of 1973 when Fix was at ICASE. The problem concerns the mixing of a supersonic laminar jet with a subsonic cross flow. For viscous compressible flow over a two-dimensional rectangular region the steady state solution is to be obtained by the Crank-Nicholson-Galerkin method applied to the unsteady equations using primitive variables. Piecewise polynominal trial functions of total degree 3 and triangular elements are used to discretize in the space variables. This problem is being worked in conjunction with Dennis Bushnell of the Hypersonic Vehicles Division and one purpose of the study is to compare finite element methods with finite difference methods for this type of problem. An ICASE report describing the algorithm and its theory has been completed and work is continuing on implementation of a program.

Dr. Max Gunzburger jointed ICASE in September, 1973 and has been working in conjunction with Lucio Maestrello of the Acoustics and Noice Reduction Division. The current problem under consideration is the propagation of sound through a realistic subsonic jet flow field. A point acoustic source is placed in the potential core of the jet. The sound emanating from this source encounters a non-homogeneous media, i.e., the jet flow field, and therefore the sound propagates in a non-uniform manner. Governing equations for the acoustic variables are derived by linearizing the Euler equations about the mean jet flow. Information about the mean jet flow is supplied by experimental measurements. The governing system for the acoustic variables is being solved

numerically by a Galerkin type method somewhat similar to that used by Cooke and Fix. (Prof. Fix has also been working with Gunzburger on the numerical methods for this problem.) Here there is a coupled system of eight partial differential equations and cubic B-splines are being used for discretization of the space variables and then a leap-frog method combined with extrapolation is used for the time integration. The computer program is now in the final stages of development.

Dr. Gunzburger, as well as Drs. Aziz and Ortega, also participated in a "working seminar" with Jerry South and other members of the Theoretical Aerodynamics Branch on various questions involved in the numerical solution of transonic flow problems.

Dr. David Yen, on sabbatical leave from Michigan State University, has also been working with the Acoustics and Noise Reduction Division on a problem concerning the motions of a clamped panel excited by supersonically convected turbulence. The problem arises when one considers an aircraft in supersonic flight and wishes to predict the noises resulting from the panel motions, both radiated to the exterior and transmitted to the interior of the aircraft. Dr. Yen's main effort on this problem has been to attempt a realistic formulation and to suggest a method whereby numerical results may be obtained.

Taking the coupling with the acoustic fields into account, the panel motions are governed by a stochastic integro-differential equation. The kernels of the integrals have been identified as Green's functions for sound radiations under various moving point and line sources and have been determined with the aid of integral transform methods. The integro-differential equation is being solved by a Galerkin method, using the plate eigenfunctions when couplings with the acoustic fields are absent.

Dr. Yen has also been continuing his research on non-linear waves in elastic plates. He is presently investigating numerically, using a finite difference method, the steady-state wave forms for nonlinear waves generated by moving loads on the plates.

Ms. Virginia Jordan, who joined ICASE on a part-time basis in September 1974, has been studying the time dependent reflection of long waves by bottom topography. A forthcoming ICASE report on this problem shows how the front of a tsunami wave train is modified by variations in the bathymetry. This effect may be the mechanism for introducing the frequencies which cause the excitation of the harbor and island resonances directly responsible for the destructive run-up effects of tsunamis. In addition, if the topography has periodic variations of the proper frequency ratio to that of the incident wave, there is the possibility of relatively large reflection of energy away from the direction of propagation.

In conjunction with Charles Whitlock of the Space Applications and Technology Division, Ms. Jordan has also been working on methods of predicting the growth and decay of the ocean wave spectrum when the wind history is known, and has also been consulting with Wade D. Morris and Lamont Poole in the same Division on questions connected with extending a program for calculating the refraction of storm waves approaching the coastline.

# 3. Other ICASE Activities

ICASE has continued to sponsor an active lecture and visitor program; a complete list of the speakers and the titles of their lectures is given in Appendix C. All of the visiting speakers participated in discussions with Langley staff members during their visit and some (e.g. Prof. Lynch) stayed over for an extra day or two of consultation. Regular ICASE members have also carried on an active program of consultation with Langley personnel in addition to the longer term collaborative efforts described in the previous section.

In June of 1973, ICASE sponsored the First Langley Conference on Scientific Computing in conjunction with the 1973 National Meeting of the Society for Industrial and Applied Mathematics (SIAM). Preparations are now under way to hold the Second Langley Conference on Scientific Computing at Virginia Beach, VA on October 21 and 22, 1974, with the theme Numerical Methods for Parallel and Vector Processors. This conference will again be cosponsored by SIAM.

Various ICASE members have been involved in one way or another with the local universities. Dr. Rosenbaum taught a graduate course in Numerical Solution of Ordinary Differential Equations at William and Mary in the Fall semester. As part of the course, the students developed a general purpose interactive ordinary differential equations program. Dr. Gunzburger is teaching a graduate course on Fluid Dynamics in the current Spring Semester. Dr. Ortega has become the co-thesis advisor for the Ph.D. work of Mr. J. Lambiotte of ACD at the University of Virginia.

Dr. Ortega has also coordinated a series of monthly meetings between representatives of three local universities in order to enhance cooperation and coordination in their programs in computer science and applied mathematics. The regular representatives have been Dr. A. Sidney Roberts, Assistant Dean of Engineering at Old Dominion University; Dr. John E. Selby, Graduate Dean of Arts and Sciences at the College of William and Mary; and Dr. John Whitesides, Coordinator of the George Washington University program at Langley. In addition, several other faculty members of the three institutions have participated in some of the meetings. One item of current interest to the group is the possibility of closed circuit television between the three locations and also Wallops Island; this would allow a more efficient sharing of courses and faculty. It is planned to continue regular meetings of the group for the foreseeable future.

## I Permanent Staff

James M. Ortega, Director Ph.D., Mathematics, Stanford University, 1962 Numerical Analysis

Robert G. Voigt, Assistant Director Ph.D., Mathematics, University of Maryland, 1969 Numerical Analysis

John C. Tredennick, Executive Assistant

Myrtle H. Wells, Secretary

## II Advisory Committee

Bruce W. Arden, Professor and Chairman of Computer Science and Electrical Engineering, Princeton University.

Samuel D. Conte, Professor and Chairman of Computer Science, Purdue University.

Eugene Isaacson, Professor of Mathematics, Courant Institute, New York University.

Randal M. Robertson, Dean, Research Division, Virginia Polytechnic Institute and State University.

# III Term Appointments

Alan K. Cline - Ph.D., Mathematics, University of Michigan, 1970. Computational linear algebra and approximation theory. Joined ICASE September, 1973.

Max D. Gunzburger - Ph.D., Mathematics, New York University, 1969. Fluid dynamics and numerical solution of partial differential equations. Joined ICASE September, 1973.

W. Terry Hardgrave - Ph.D., Computer Science, University of Texas at Austin, 1972. Data management and operating systems. Joined ICASE in January, 1974.

Virginia S. Jordan - Ph.D., Applied Mathematics, Harvard University, expected 1974. Differential equations and fluid dynamics. Joined ICASE in September, 1973 on part-time appointment while completing thesis.

Richard C. Raffenetti - Ph.D., Physical Chemistry, University of Iowa, 1971. Postdoctoral fellow, Batelle Institute. Computational chemistry. Will join ICASE in March, 1974.

Jerrold S. Rosenbaum - Eng. Sc.D., Applied Mathematics, Columbia University, 1971. Numerical solution of ordinary differential equations. Joined ICASE, August, 1973.

## IV Visiting Scientists

A. Kadir Aziz - Ph.D., Mathematics, University of Maryland. 1958. Professor of Mathematics at the University of Maryland at Catonsville. Nonlinear partial differential equations and finite element methods for gas dynamics problems. At ICASE from September 1, 1973, to June 1, 1974.

Victor B. Basilli, Ph.D., Computer Sciences, University of Texas at Austin, 1970. Assistant Professor of Computer Sciences, University of Maryland. Programming languages and compiler construction. At ICASE one week in summer of 1974.

James C. Browne - Ph.D., Physics, University of Texas at Austin, 1960. Professor and Chairman of Computer Science and Professor of Physics at the University of Texas at Austin. Operating Systems. At ICASE June 1 - August 1, 1974.

Goerge J. Fix - Ph.D., Mathematics, Harvard University, 1968. Associate Professor of Mathematics at the University of Michigan. Numerical methods for partial differential equations and, in particular, finite element methods for fluid dynamics. At ICASE, December 17-21, 1973, and again May 1 - September 1, 1974.

Alan George - Ph.D., Computer Science, Stanford University, 1971. Assistant Professor of Computer Science, University of Waterloo. Numerical linear algebra and finite element methods. At ICASE December 3-17, 1973, and then for May 1 - August 1, 1974.

C. William Gear, Ph.D., Mathematics, University of Illinois, 1960. Professor of Computer Sciences and Applied Mathematics, University of Illinois. Numerical solution of ordinary differential equations. at ICASE June 17 - June 28, 1974.

Gene H. Golub - Ph.D., Mathematics, University of Illinois, 1959. Professor of Computer Science at Stanford University. Large-scale matrix problems and numerical solution of partial differential equations. At ICASE September 6-13, 1973, December 11-13, 1973, and additional short visits in future.

Bertil Gustafsson, Ph.D., University of Uppsala (Sweden), 1968, Acting Professor of Computer Science, University of Uppsala. Numerical solution of partial differential equations. At ICASE July 1, 1974 - June 30, 1975.

John C. Knight - Ph.D., Computer Science, University of Newcastle-Upon-Tyne, 1974. Assistant Professor of Computer Science at the University of West Virginia. Virtual and paged memories, especially for the STAR. At ICASE for January 3-11, 1974, and then for the summer of 1974.

Jorge J. More - Ph.D., Mathematics, University of Maryland, 1970. Assistant Professor of Computer Science at Cornell University. Numerical analysis and optimization. At ICASE for the summer of 1974.

Steven Orszag, Ph.D., Physics, Princeton University, 1966. Associate Professor of Applied Mathematics, Massachusetts Institute of Technology. Comptational fluid dynamics. At ICASE for one or two weeks in July, 1974.

William G. Poole, Jr. - Ph.D., Computer Science, University of California at Berkeley, 1970. Assistant Professor of Mathematics at the College of William and Mary. Development of algorithms for vector processors. At ICASE from September 1, 1973, to June 1, 1974, and then half time in summer of 1974.

Gerald R. Richter, Ph.D., Applied Mathematics, Harvard University, 1971. Assistant Professor of Mathematics, University of Michigan. Numerical solution of partial differential equations. At ICASE for summer of 1974.

Stephen W. Sherman - Ph.D., Computer Science, University of Texas at Austin, 1972. Assistant Professor of Computer Science at the University of Houston. Operating Systems. At ICASE January 7-11, 1974, and then will rejoin ICASE on 15-month appointment, June 1, 1974.

Harold Stone, Associate Professor of Computer Science and Electrical Engineering, Stanford University. Parallel processing. At ICASE May 13-17, 1974.

David H. Y. Yen - Ph.D., Mathematics, New York University, 1965. Professor of Mathematics and Metallurgy, Michigan State University. Engineering Mechanics. At ICASE January 1 - June 30, 1974.

# V Student Assistants

Susan M. McCabe - B.S., Mathematics, William and Mary College, 1973. Graduate student at William and Mary. Working half time at ICASE since September 1, 1973.

# Appendix B.- Reports and Publications

- 1. Sherman, Stephen W.: Suggestions of Operating System and Software Improvements for ICOPS. September 4, 1973.
- 2. Sherman, Stephen W.: A Trace-Driven Model of the Integrated Computer Operating System at NASA Langley. September 26, 1973.
- 3. Poole, William G., Jr.: Expected Pivot Size in Gauss Elimination. October 19, 1973.
- 4. Cooke, Charlie H.; and Fix, George J., III: A Finite Element Solution Algorithm for the Two-Dimensional Compressible Navier-Stokes Equations. November 29, 1973.
- 5. Fix, George J., III: Finite Element Approximation of Ocean Circulation Problems. December 11, 1973.

- Appendix C.- <u>ICASE Seminar Program</u> <u>September 1, 1973 - February 28, 1974</u>
- September 7, 1973 Prof. Gene H. Golub, Computer Science Department, Stanford University; "Solution of Nonlinear Least Squares Problems"
- September 24, 1973 Panel Discussion "Trends in Computer Hardware and Software"

  Prof. James C. Browne, University of Texas at Austin; Dr. R. Stockton Gaines, Institute for Defense Analyses, Princeton, NJ; Prof. Saul Rosen Purdue University; Prof. Stephem W. Sherman, University of Houston
- September 27, 1973 <u>Dr. Michael D. Cox</u>, Geophysical Fluid Dynamics Laboratory, Princeton, NJ; "A Numerical Model for Oceanic General Circulation"
- October 1, 1973

  Prof. Richard H. Bartels, Computer Science Department, University of Texas at Austin; "Nonlinear Least Squares Without Derivatives"
- October 10, 1973 Prof. Joseph F. Traub, Computer Science Department, Carnegie-Mellon University; "Parallel Algorithms"
- October 18, 1973 Dr. Alan K. Cline, ICASE; "Applications of Splines Under Tension"
- October 25, 1973 <u>Dr. Jerrold S. Rosenbaum</u>, ICASE; "Numerical Methods for Stiff Systems"
- November 1, 1973 Dr. William J. Quirk, NASA Institute for Space Studies, New York; "Energetics as a Diagnostic Tool for Global Circulation Models"
- November 12, 1973 Prof. C. C. Paige, Computer Science Department, McGill University, Montreal; "The Lanczos Process, Eigenvalues, and Solutions of Linear Equations"
- November 20, 1973 Prof. William G. Poole, ICASE and College of William & Mary; "Large Sparse Linear Systems"
- November 30, 1973

  Prof. Thomas E. Hull, Computer Science Department,
  University of Toronto, Canada; "Structure, Reliability and Efficiency of Programs for Solving Ordinary
  Differential Eugations"
- December 4, 1973

  Prof. Alan George, Computer Science Department,
  University of Waterloo; "On the Use of the Woodbury
  Formula to Solve Sparse Linear Systems"

- December 11, 1973 Dr. Charles Van Loan, Department of Mathematics, University of Michigan; "Generalized Singular Values: Theory, Algorithms, and Applications"
- December 17, 1973 Prof. Robert E. Noonan, Computer Science Department, University of Maryland, College Park; "A Canonical Form for Computer Programs"
- December 18, 1973 Prof. Richard F. Sincovec, Computer Science Department, Kansas State University; "The Numerical Method of Lines for the Solution of Nonlinear Partial Differential Equations"
- December 20, 1973 Prof. Alexandre Chorin, Mathematics Department, University of California at Berkeley; "Random Elements and Stochastic Approximations in Turbulence Calculations"
- January 2, 1974 <u>Dr. David Gottlieb</u>, Department of Mathematics, MIT;
  "A Fourth Order Finite Difference Scheme for the Equations of Gas Dynamics in Two and Three Space Dimensions"
- January 8, 1974 <a href="Prof.W.C. Lynch">Prof. W. C. Lynch</a>, Computing and Information Science, Case Western Reserve University; "The Dynamics of Virtual Memory Systems"
- January 14, 1974 <u>Dr. Terry Hardgrave</u>, ICASE; "Set Theory in Generalized Data Management Systems"
- January 18, 1974 Prof. David H. Y. Yen, Michigan State University and ICASE; "Wave Motions in Continuous Media Generated by Moving Disturbances"
- January 25, 1974 <u>Dr. David G. Korn</u>, Courant Institute of Mathematical Sciences, New York University; "Transonic Aerodynamics"
- February 4, 1974 Mr. Michael Steuerwalt, Computer Science Department,
  University of Wisconsin, Madison; "Computational Solution
  of Mildly Nonlinear Elliptic Boundary Value Problems with
  Multiple Solutions"
- February 13, 1974 Dr. Ivan E. Sutherland, Evans & Sutherland Computer Corp., Salt Lake City, Utah; "Dynamic Computer Graphics in Three Dimensions"

# INSTITUTE FOR COMPUTER APPLICATIONS IN

SCIENCE AND ENGINEERING (ICASE)

Semi-Annual Report

March 1, 1974 - August 31, 1974

#### 1. The ICASE Research Program

The major categories of the ICASE research program are:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR series.
- b. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
- c. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.
- d. Computer systems and software.

The work in each of these areas will be described briefly in this section, while other activities are discussed in Section 2.

## a. Efficient Use of Vector and Parallel Computers

Dr. Robert G. Voigt, Assistant Director of ICASE, has devoted most of his activity apart from administrative duties to this area. He and Mr. J. J. Lambiotte of the Analysis and Computations Division (ACD) finished a joint ICASE report on the best ways to solve tridiagonal systems of equations on vector and parallel computers, and the STAR computer in particular. This work was described in more detail in the previous semi-annual report. Dr. Voigt presented the results at an ICASE seminar and the paper has been submitted for publication in the ACM Transactions on Mathematical Software.

Professor William G. Poole spent the year September 1, 1973 August 31, 1974 at ICASE on leave from William and Mary College. He and
Dr. Voigt completed an annotated bibliography on numerical methods for
vector and parallel machines. This contains over 100 references to papers

and reports (many unpublished) on numerical methods, and is believed to be complete as of the date of publication. It also contains almost 100 additional references on closely related subjects. The bibliography has appeared as an ICASE report, and has been accepted for publication in Computing Reviews.

Poole and Voigt also are working on a gaussian elimination program for linear equations using an adaptive pivot strategy. The goal is that interchanges, a relatively costly operation on STAR, would not be required nearly as often as with the usual partial pivoting strategy particularly when a solution of only a few digits accuracy is acceptable.

A major cooperative effort between the Structures and Dynamics Division, ACD, George Washington University (GWU) and ICASE was begun in January, 1974 with the goal of producing a pilot finite element program (FESS) for the STAR. Dr. James M. Ortega of ICASE assisted Prof. A. Noor of GWU in the organization of the work and various ICASE people are cooperating on certain aspects of the problem; in particular, Dr. Poole has primary responsibility in the development of the numerical methods. Fairly detailed specifications of the program have been produced, but further work is awaiting clarification of the delivery date of the STAR.

Dr. Alan Cline, who is at ICASE on a term appointment which has been continued to September, 1975, continued his investigation of Lanczos method for the solution of large systems of linear equations. This method seems particularly suited to the STAR vector and sparse vector capability. However, the basic convergence and stability properties of the method are not yet understood on sequential machines and Cline has been carrying out a mathematical analysis as well as extensive numerical testing on the 6600.

Tests were performed using matrices supplied by Robert Camin of GWU and Sharon Padula of the Acoustics and Noise Reduction Division. The tests used the unsymmetric Lanczos method with residual minimization as well as the conjugate gradient and symmetric Lanczos methods. Uniformly, it was found that the required number of iterations (for only several places of accuracy) nearly equaled or grossly exceeded the order of the system. (Prof. A. George of the University of Waterloo has reported similar results). A "block" Lanczos algorithm using several vectors was defined, programmed and initial tests performed. Its advantages are i) Maintenance of orthogonality, ii) Acceptance of multiple right hand sides, and iii) Possibly more efficient use of the operator application. Testing is still underway as is the formulation of a minimum residual block algorithm, but preliminary indications are that, without further modification, any Lanczos algorithm will require at lease the same number of iterations as the order. Work on this project is continuing.

Mr. Don Heller, a Ph.D. student of Prof. J. Traub at Carnegie - Mellon University, spent the summer at ICASE. He first completed some work begun at Carnegie-Mellon on a unified technique for parallel computation of linear recurrences. This appeared as an ICASE report and was submitted for publication in the IEEE Transactions on Computers. For the balance of the summer, Heller investigated the use of a cyclic reduction algorithm for block tridiagonal linear systems. The method considered is an extension of one used by Lambiotte and Voigt for tridiagonal systems. Under conditions of diagonal dominance, matrix norms of the off-diagonal blocks decrease quadratically relative to the diagonal blocks with each reduction. This allows a possibly early termination of the reduction. An ICASE report

on this work was completed and will be submitted for publication in the SIAM Journal on Numerical Analysis.

Many of the above activities have been stimulated by, and coordinated with, the work of ACD through a series of meetings of a "STAR Linear Algebra Working Group" consisting of several members of both ICASE and ACD. They were also stimulated by a week's visit by Prof. Harold Stone of Stanford University.

Dr. John Knight spent the first part of the summer at ICASE prior to accepting a permanent NASA position in ACD on August 1. Apart from general consultation with ACD, Dr. Knight was involved in two research projects. The first was in collaboration with Drs. Poole and Voigt on an analysis of the balance between I/O and numerical computations on the STAR. The problem considered was the solution of banded systems of linear equations so large that the problem can not be core-contained.

The results are probably the first of this type which have been obtained for a STAR class machine, and have proved useful in assessing the suitability of various configuations for the STAR, in determining operating system strategy, and in evaluating peripheral devices. Now under consideration are more difficult types of linear systems such as arise in finite element codes using "substructuring". It is expected that the study will have a direct impact on the FESS project mentioned above.

Dr. Knight also collaborated with Prof. Victor Basili of the University of Maryland on defining a new high level programming language for the STAR. Such a language would be an alternative to the extended Fortran language to be supplied with the STAR and would have several advantages over Fortran, especially in regards to accessing STAR hardware

instructions. This new language, currently known as SL/1, has a careful selection of data types and data structures, and provides a set of operators which closely match the machine's hardware instructions. In this way, the user is able to write programs which access the special hardware directly. Work on this project is continuing.

## b. Numerical Analysis

In this section, we will review work done in the analysis and development of numerical algorithms with no particular emphasis on the STAR computer. It should be recognized, however, that many times there is no clear dividing line between the two efforts.

Dr. Poole, in collaboration with Profs. N. Gibbs and P. Stockmeyer of William and Mary, was able to extend the results on bandwidth reduction of large sparse matrices discussed in the previous semi-annual report. The extension was to profile reduction as follows. In a banded matrix, it may happen that some rows have leading zero elements within the band and this fact can be utilized in reducing computation time as well as storage in the factorization of such matrices. The profile reduction problem is then analogous to that of bandwidth reduction: to permute the rows and columns of the matrix in such a way as to obtain a new matrix with a minimal, or at least greatly reduced, profile. Poole, et.al. were able to use their techniques for bandwidth reduction in order to obtain corresponding algorithms for profile reduction. This work was incorporated in the report on bandwidth reduction. It was discussed in an ICASE seminar by Dr. Poole, issued as a joint ICASE and William and Mary report, and submitted for publication to the SIAM Journal on Numerical Analysis.

The program for carrying out these reductions will be documented in a subsequent report and be submitted for publication in the ACM Transactions on Mathematical Software.

Two further aspects of this project on bandwidth and profile reduction are currently being pursued by Gibbs, Poole, and Stockmeyer. The first is a comprehensive testing program for several reduction algorithms; it is hoped that a clear method of choice will result from this work. The second is a modification of an algorithm due to King for profile reduction. This algorithm can give smaller profiles than the algorithm of Cuthill-McKee, but one does not know the best way to start the algorithm. It is hoped that this problem can be overcome.

Dr. Alan Cline, in conjunction with J. F. Walsh of the National Center for Atmospheric Research, completed the development of a collection of subroutines for performing regression analysis. This work, which was begun at NCAR, was issued as an ICASE report, was presented by Dr. Cline at the Purdue Conference on Mathematical Software in May, 1974, and has been submitted to the ACM Transactions on Mathematical Software.

In preparing for publication the algorithm for finding the best uniform approximate solution of an overdetermined linear system of equations, which was described in the previous semi-annual report, Dr. Cline discovered more elegant ways of handling the analysis of the algorithm. This necessitated a delay in the completion of the work, but an ICASE report has now been finished and will be submitted for publication in the SIAM Journal on Numerical Analysis. Cline also presented these results at an ICASE seminar.

Dr. Cline gave a short course at ICASE during June 17-28, 1974 on "Theory and Application of Singular Values". The singular values of a matrix are related (in concept) to the eigenvalues of a matrix and are useful in a variety of problems in computational linear algebra. The course had an enrollment of over 20 NASA and other people. The notes for the course are now being written up as an ICASE report which will be submitted as a survey paper to the SIAM Review. Some additional research results on perturbation theory of singular values will form a second report.

Dr. Cline also began research on two new algorithms for computing the eigenvalues and vectors of matrices. The first is a highly parallel method which may be valuable for the STAR. Essentially it exploits the fact that the singular values of a symmetric matrix are the absolute values of the eigenvalues and that a highly parallel (or vectorizable) algorithm for singular value decomposition can be defined using the biorthogonalization idea of Hestenes. No programs or testing have been done yet however. The second algorithm, for the generalized eigenvalue (and singular value) problem has been defined but not tested. The algorithm maintains the symmetry of the matrices and requires a very low number of operations when compared to the QZ algorithm. Work on both of these algorithms is continuing.

Some of the above work of Cline, Poole, and Voigt was reviewed by Prof. Gene H. Golub of Stanford University during his visit of August 26-28. This in turn led to some ideas for further research which is now under consideration.

Prof. J. Alan George of the University of Waterloo spent the period May 1 - August 1 at ICASE. His research during this period centered

on two main problems. The first was aimed at producing an algorithm for solving finite element equations arising from two dimensional irregular meshes in  $O(N^{3/2})$  operations, where N is the number of vertices in the finite element mesh. There are strong reasons for believing that this is optimal for problems which are really two dimensional (i.e. the number of vertices on the edge of the mesh is much smaller than the number of interior vertices). A code was developed to study various ordering strategies, and although several strategies appear to produce an  $O(N^{3/2})$  ordering, he has not as yet been able to prove that any of these strategies <u>must</u> produce such an ordering for general finite element meshes. Prof. George will continue this work at Waterloo.

The second project was an investigation of methods related to that of Kron - so-called methods of matrix tearing and modification. The basic idea is to attempt to solve a given sparse matrix problem Ax=b by solving one or more "nearby" problems (in the sense of sparsity) which are much easier to solve. One pays a price for these easier problems; one must somehow recover the solution to the original problem. The object of George's investigation was to attempt to determine if and/or when these various strategies actually result in a net saving in operations and/or storage. The results so far are scattered. One ICASE report summarizing some negative results was completed and submitted to the SIAM Journal on Numerical Analysis. A second report is in preparation.

Prof. A. Kadir Aziz, on leave from the University of Maryland, completed his nine-month stay at ICASE on May 31. During this period, he investigated the application of the finite element method to hyperbolic and mixed hyperbolic-elliptic partial differential equations. A major part of this effort was directed to the study of equations of the form

 $g(x,y)\phi$  + $\phi$  = f where g can change sign in the domain of the problem. Considerable progress was made both in questions of existence and uniqueness of solutions of the differential equation as well as in the theory of finite element methods as applied to such equations. This work appeared in part as an ICASE report which will be submitted for publication in Mathematics of Computation.

Prof. Gerard Richter of the University of Michigan spent the period June 1 - August 1, 1974 at ICASE, supported in part by an NSF Grant. His specialty is numerical solution of integral equations and he worked during the summer primarily on equations of the first kind in response to questions raised by several NASA people. He also gave a survey lecture on such problems. The basic difficulty presented by Fredholm integral equations of the first kind is that of instability: small perturbations in the problem may lead to arbitrarily large changes in the solution or produce a problem without a solution. This is particularly crucial from a practical standpoint since measurement error is typically inherent in the problem and roundoff and truncation error are inevitably incurred in the computation of the solution. Several methods for "stabilizing" the solution were studied and brought to the attention of interested NASA people. Somewhat surprisingly computational evidence developed by Prof. Richter suggested that the Nystrom method and Galerkin's method when applied to Fredholm integral equations of the first kind with smooth solutions, produce the desired order of convergence (e.g. 0(h2) for piecewise linear approximation), provided measurement and roundoff errors do not contaminate the numerical solution. An attempt was made to prove this conjecture, but at this point it remains an open question.

Prof. Jorge More of Cornell University spent the period

June 1 - August 1 at ICASE with half-time support from an NSF grant.

During the period he worked primarily in collaboration with Prof. A. Noor of George Washington University on an investigation of methods which are suitable for solution of large sparse systems of nonlinear equations such as arise in finite element analysis of structures. In particular, the methods of Brown and Broyden were considered for these problems, but were found to be rather unsuitable in their present form. Ultimately, a subroutine for the nonlinear Gauss-Seidel method was implemented and left with Prof. Noor. The results of this study were summarized at an ICASE seminar. Dr. More also continued work on a survey paper about the use of quasi-Newton methods for nonlinear equations and unconstrained optimization problems. This work is being done in collaboration with Prof. John Dennis of Cornell University.

Prof. George Fix of the University of Michigan spent the period May 15 - August 21 at ICASE, also supported in part by an NSF grant.

During this period he worked on a number of problems, most of which are discussed in the next section. In numerical analysis, he developed a new approach to using the SOR iteration for elliptic boundary value problems discretized on a grid with variable spacing. The idea is to use relaxation factors which vary over the grid points (but are fixed with respect to the iteration number). Fix showed that there is an optional set of such parameters, which unfortunately is too costly to compute. However, using the closure arguments of Garabedian, he was able to estimate these parameters efficiently. Limited numerical experiments using these estimates have been very encouraging. Work is continuing on the project and an

ICASE report will be completed in the future.

Prof. Fix also worked in conjunction with Dennis Jespersen, a graduate student at the University of Michigan who spent the period July 11 - August 31, 1974 at ICASE, on investigating the errors in finite element approximations of degenerate elliptic problems. These cases arise when viscosities (or diffusivities) vanish at the boundaries. The central issue is to understand what effects are created in the accuracy in interior subregions. This work will continue during the following academic year at the University of Michigan.

Dr. Jerrold Rosenbaum, who has been at ICASE on a term appointment since August 1973 and will continue until June 1975 on a half-time basis, has been continuing with his research on the numerical solution of stiff systems of ordinary differential equations that was outlined in the last semi-annual report. He has shown that if a system of differential equations represents a property conserving system which can be expressed linearly (e.g. conservation of mass) then numerical methods such as Runge Kutta and linear multistep methods preserve the same linear quantity and Newton type methods used for solving the implicit equations preserve the conservation property of the numerical methods. This work has been described in an ICASE report which will be submitted for publication to the Journal of Computational Physics.

Together with Dr. R. Bowles of ACD, Dr. Rosenbaum is investigating real time integration of differential equations. The numerical implementation of the local linearization algorithm (developed by Bowles et al.) is being considered. Dr. Rosenbaum has also found a way to implement implicit integration processes in real time. Work on this project is continuing.

Prof. G. William Gear of the University of Illinois spent the period June 17 - 28, 1974 at ICASE and began a collaboration with Dr. Bowles and Dr. Rosenbaum on the above real-time simulation problem. Gear and Rosenbaum are currently preparing a prospectus of work to be done in this area over the next several months.

## c. Computational Research in Science and Engineering

Prof. Fix continued his collaboration with Prof. Charles Cooke of Old Dominion University on the use of finite element methods for fluid flow problems. This project is being done in conjunction with the High-Speed Aerodynamics Division and was described in the previous semi-annual report. Considerable progress was made in debugging the program and overcoming various problems which arose. Numerical experiments are continuing and it is hoped that an ICASE report on this work will be completed in the near future.

Prof. Fix also continued work on the limited region ocean circulation model which was described in the Annual Report of September 1973 and in an ICASE report of August 27, 1973. A paper by Prof. Fix on this work is scheduled to appear shortly in the SIAM Journal on Applied Mathematics and he has been continuing his collaboration with Drs. J. Hirsch and A. Robinson of Harvard University on numerical computation using the model.

Dr. Max Gunzburger, who is on a term appointment at ICASE which has been continued to September 1975, has been working primarily in conjunction with Lucio Maestrello of the Acoustics and Noise Reduction Division (ANRD). The main problem that Dr. Gunzburger has considered is unsteady propagation of sound through a realistic subsonic jet flow field. A point acoustic source is placed in the potential core of the jet. The sound

emanating from this source encounters a non-homogeneous media, i.e., the jet flow field, and therefore the sound propagates in a non-uniform manner. The governing equations for the acoustic variables are derived by linearizing the Euler equations about the mean jet flow and are being solved by a semi-discrete method in which the space dependence is approximated by Galerkin's method using cubic B-splines. This yields a system of ordinary differential equations governing the time dependence. A computer program has been written and debugged. However, unforeseen difficulties in the numerical treatment of the problem has for the present prevented the program from successfully finding solutions. Presently, the program is undergoing revisions and testing after consultation between Dr. Gunzburger and other members of the TCASE staff, most notably Prof. Fix.

Also in collaboration with Maestrello and Dr. C. H. Liu of the ANRD and Prof. Lu Ting of the Courant Institute, Dr. Gunzburger has worked on two other problems. The first is the propagation of sound through a turbulent jet. This problem has been formulated in terms of correlations of primitive acoustic variables. The formulation of the problem, and a numerical scheme for its solution, has resulted in an ICASE report by Gunzburger, Liu, Maestrello, and Ting and the work was also presented by Mr. Maestrello at an AIAA meeting. The second problem is the modeling of a turbulent subsonic jet by randomly releasing ring vortices. A computer program is being written by Dr. Liu which uses a theory and programs previously developed by Dr. Gunzburger. Dr. Gunzburger is assisting in the development of the model and the resulting program.

Prof. Fix and Dr. Gunzburger collaborated on a study of various boundary conditions that can be imposed on the outflow region in fluid

problems. They have shown that the usual downstream continuation is (weakly) unstable for standard difference schemes. To counter this they have proposed integral boundary conditions which are stable. Numerical experiments are currently being carried out using the linearized Burger equation as a simple model. This work, which should have potential application to a number of fluids problems at Langley and elsewhere, is being documented in an ICASE report and will be presented in an invited lecture by Prof. Fix at the forthcoming First International Symposium on Computational Methods in Nonlinear Mechanics.

Drs. Fix, Gunzburger, and Rosenbaum collaborated on a problem originally motivated by the work of Dr. R. Boughner and others of the Space Systems Division in their study of the modeling of chemical kinetic transport in the atmosphere. This problem has application to stratospheric pollution caused by the SST or space shuttle and involves the numerical solution of a system of non-linear partial differential equations in time and one or more space variables. A previous computation with no space variables (i.e. a system of ordinary differential equations which are stiff because of the chemical reactions) has been done by Dr. Boughner, with consultation from Dr. Rosenbaum. For one space variable, Dr. Boughner has pursued a finite difference approach and the initial purpose of the ICASE effort was to investigate the feasibility of using finite element methods for this problem; these high order methods could be potentially very useful for two or three space variables. The first step has been to repeat the one space variable calculations using a Galerkin approach with cubic splines. Comparisons between this and the finite difference scheme can then be made. The program is being written by Mr. Martin Cordes, a summer student at ICASE.

Prof. David Yen was at ICASE from January 1, to June 30, 1974 while on sabbatical leave from Michigan State University. Dr. Yen worked with the Acoustics and Noise Reduction Division on a problem concerning the motions of a clamped panel excited by supersonically convected turbulence. The problem arises when one considers an aircraft in supersonic flight and wishes to predict the noises resulting from the panel motions, both radiated to the exterior and transmitted to the interior of the aircraft. Dr. Yen's main effort on this problem was to attempt a realistic formulation and to suggest a method whereby numerical results might be obtained. Taking the coupling with the acoustic fields into account, the panel motions were governed by a stochastic integro-differential equation. The kernels of the integrals were identified as Green's functions for sound radiations under various moving point and line sources and determined with the aid of integral transform methods. A Galerkin method, using the plate eigenfunctions in the absence of the acoustic couplings as the base functions, was suggested for solving the governing integro-differential equation. Numerical results are still being obtained and analyzed and Dr. Yen plans to continue collaboration with ANRD during the following year.

Dr. Yen aled worked on a problem concerning the periodic motions in a class of nonlinear systems with two degrees of freedom and developed a numerical method for determining such motions. The method grew out of his previous work in which properties of such periodic motions were investigated theoretically. Numerical results, obtained for some example systems involving linear, cubic and quintic spring forces, support the theoretical predictions of Dr. Yen and reveal further details on the properties of the

periodic motions. The results are contained in an ICASE report, and a condensed version of the report will also appear in the Proceedings of the First International Symposium on Computational Methods in Nonlinear Mechanics.

Dr. David Gottlieb, of the Massachusetts Institute of Technology, spent the period June 1 - August 31, 1974 at ICASE. He and Prof. Bertil Gustafsson, who is spending the year July 1, 1974 - July 1, 1975 at ICASE on leave from the University of Uppsala (Sweden), collaborated on a project with Dr. Julius Harris and others of the Fluid Mechanics Branch of HSAD. The problem under consideration is the determination of the flow in a domain with an incoming supersonic jet. The mathematical model is a modified version of the Navier-Stokes equations in two space dimensions. The methods currently being used for reaching steady state converge too slowly or do not converge at all in certain parts of the domain. A fundamental difficulty is the necessary introduction of artificial boundaries. The linearized system of differential equations with second order derivatives neglected has been analyzed and well-posedness proved for the initial value problem. An interesting fact is that the characteristic speeds are not the same as for the system obtained from the full Navier-Stokes equations. This will effect among other things the way of posing boundary conditions. The well-posedness of the initial boundary value problem has been considered but the analysis is not yet completed. The aim is to apply a difference scheme of the leap-frog, Du Fort-Frankel type with fourth order accurate operators in space. For this purpose, the second order Du Fort-Frankel scheme has been generalized to arbitrarily high order accuracy in space. Stability for the initial value problem has been proved for a general parabolic system

in two space dimensions assuming symmetric coefficient matrices. This has not been proved before even for the second order accurate Du Fort-Frankel scheme. This project will continue during the next several months.

Dr. Gustafsson also began investigating a problem of interest to Gerald Wahlberg and Kenneth Sutton of the Advanced Entry Analysis Branch. This is the problem of calculating the flow about axisymmetric blunt bodies at hypersonic speed. The governing mathematical model is a system of nonlinear hyperbolic equations. Presently used methods for obtaining steady state use explicit difference schemes applied to this system. The calculations at each time step are very time consuming and a more efficient method of solution is desired. One approach is to use an implicit difference method for the time dependent equations, thereby being able to use large time steps. Another approach is to solve the discretized version of the steady state systems. In both cases large systems of nonlinear algebraic equations must be solved efficiently. A quasi Newton method will probably be efficient. To gain insight a one dimensional version of the system was analyzed, and an approximation of the box-type scheme was defined. Numerical experiments have been done, and a fairly good convergance rate was obtained. However, further experiments must be done before any conclusions can be made. Work on this project is continuing.

Dr. Gottlieb also considered a different approach to high order methods for hyperbolic equations. In a recent paper, H. Kreiss and J. Oliger have shown the superiority of fourth order approximations for the space variables in hyperbolic problems. However, the natural extension of the well-known Lax-Wendroff scheme to fourth-order accuracy gives a very bad stability condition and J. Gary has recently shown that it is impossible to reformulate it in two time steps. Dr. Gottlieb has used another approach

to construct a fourth-order two step Lax-Wendroff scheme with a better stability condition. This method is dissipative of order 6 and can be generalized easily to any number of dimensions. Dr. Gottlieb plans to continue this investigation over the next several months while at M.I.T.

Prof. Micha Wolfshtein joined ICASE on August 18, 1974 for a one-year stay while on sabbatical leave from the Technion in Israel, and will do research on turbulence modeling. Most existing models of turbulence inherently imply that the spectral distribution of turbulent quantities has only a negligible influence on the development of the flow field. However, this assumption does not appear to be realistic in some important cases. Typical examples are: (i) the strong influence of the frequency of sound waves on the spread of free mixing layers; (ii) the high sensitivity of stagnation flow to the spectral distribution of the turbulence in the oncoming stream; and (iii) the significant reduction in drag in boundary layers on complian + Alls. These phenomena cannot be satisfactorily explained by the existing mean frequency theories. Prof. Wolfshtein is planning to develop a new model of turbulence (applicable to shear flows) in which the turbulence will be assumed to depend on the frequency distribution of the variables as well as on the spatial and temporal coordinates. Such a model will not require a length scale equation, but, on the other hand, the number of dimensions of the variable space will be increased, as the one or three dimensional wave number will become now a coordinate as well. It is hoped that this work will yield the governing model equations as well as a numerical method for their solution.

Ms. Virginia Jordan was at ICASE from September 1. 1973 to June 1. 1974 on a part-time appointment. During this period, she studied the time dependent reflection of long ocean waves by bottom topography and showed how the front of a tsunami wave train is modified by variations in the bathymetry. This effect may be the mechanism for introducing the frequencies which cause the excitation of the harbor and island resonances directly responsible for the destructive run-up effects of tsunamis. addition. if the topography has periodic variations of the proper frequency ratio to that of the incident wave, there is the possibility of relatively large reflection of energy away from the direction of propagation. In conjunction with Charles Whitlock of the Space Applications and Technology Division. Ms. Jordan also worked on methods of predicting the growth and decay of the ocean wave spectrum when the wind history is known, and consulted with Wade D. Morris and Lamont Poole in the same division on questions connected with extending a program for calculating the refraction of storm waves approaching the coastline.

Mr. Micheal Ghil, a Research Associate at the Courant Institute of Mathematical Sciences, spent the month August 1 - 30, 1974 at ICASE working on a numerical method for the initialization of the equations of dynamic meteorology. This work was of interest to the Space Applications and Technology Division. For simplicity, the shallow water equations were considered and in this case the technique requires solving a large system of nonlinear algebraic equations after discretization of the differential equations. An SOR type method was used on simple test cases with some success but further work will be required to ascertain the usefulness of the method.

There were a number of other visitors in computational fluid dynamics for periods of a week or two. These were: Dr. A. Jerry Baker of Bell Aerospace Corp. who consulted with several Langley people including Dennis Bushnell, Rich Margason, and Clay Rogers; Prof. Moshe Israeli of the Massachusetts Institute of Technology, who reported on recent work in the numerical solution of ocean circulation models; Dr. Joseph Oliger of the National Center for Atmospheric Research, who consulted on various problems in the numerical solution of hyperbolic equations; and Prof. Steven Orszag of the Massachusetts Institute of Technology, who has been working on problems in connection with the Acoustics and Noise Reduction Division.

Dr. Richard Raffenetti is at ICASE on a year's appointment through March 1975 and has been working primarily in conjunction with Dr. Donald Phillips of the Environmental and Space Sciences Division on quantum chemical calculations. This involves numerical solution of the Schrödinger equation and Dr. Raffenetti has implemented at Langley two large programs developed by Raffenetti and others of Battelle Institute. These programs are now being applied to the question of the mechanisms involved in the oxidation of atmospheric nitric oxide (NO) to the pollutant nitrogen dioxide (NO<sub>2</sub>). Experimentation is difficult and only inconclusive results are available as regards the possible intermediate compound NO<sub>3</sub> and also as to whether singlet oxygen participates in a direct oxidation mechanism. Preliminary work suggests that approximate eigenvalues of a matrix of order greater than 40,000 will be required in order to obtain satisfactory conclusions.

A second problem, which is being investigated by Drs. Phillips and Raffenetti in conjunction with Dr. J. Pellet of the Space Applications

and Technology Division, is the calculation of a bond energy and the entropy of the complex H<sub>3</sub>NHCl. This complex is proposed as a key participant in natural processes leading to the removal of chlorine compounds from the stratosphere where they can act as catalytic agents for undesirable ozone decomposition. Such chlorine contamination is currently receiving much attention in connection with space shuttle research (chlorine in exhaust gases) and also because escaped freon refrigerant gases are a potential source for chlorine. Verification of a natural process of chlorine elimination is essential in order that projected shuttle flights may be carried out.

The work of Drs. Cline, Gunzburger, Gustafsson, Raffenetti, and Rosenbaum, as well as that of several others to a lesser extent, benefited substantially from the expert programming support of Ms. Susan McCabe, a graduate student at William and Mary College who was with ICASE half-time for the academic year and full-time for the summer. Her duties will be assumed by Mr. Ronald Boisvert, also a William and Mary graduate student, during the next academic year.

# d. Computer Systems and Software

Prof. Stephen Sherman of the University of Houston is spending the period May 1974 to September 1975 at ICASE. Dr. Sherman is principal investigator on a supplementary NASA grant to ICASE which has allowed the acquisition of a Prime 300 mini-computer system and associated graphics terminals. The system was installed in August, and will be used to study the potentialities of a low-cost mini-computer for interactive graphics, data base management, and a variety of other functions. The mini-computer can be either

stand-alone or connected to a larger host computer. This study is being co-sponsored by ACD and by the IPAD project of the Structures and Dynamics Division (SDD). Dr. Sherman spent a large part of the summer in preparation for the installation of the Prime and in gathering literature pertaining to distributed computing and related subjects.

Dr. Sherman also continued work on the trace-driven simulation model, discussed in the previous semi-annual report, and contributed to the implementation of the MORTRAN compiler on the CDC 6000's at ACD.

Dr. W. Terry Hardgrave, who is at ICASE on a term appointment until September 1975, continued work on a number of projects in the area of data management. He is principal investigator on a supplemental NASA grant to study the potentialities of the STDS program developed by STIS, Inc. of Ann Arbor, Michigan. This is a data management system based on concepts from set theory and Dr. Hardgrave is using the system by remote access to the Computer Center at Wayne State University. This work will continue for the next several months. Dr. Hardgrave has also begun the design of another data management system based on set theory to be implemented on the Prime 300; this work will benefit from the experience gained from use of the STDS system. Finally, a large portion of Dr. Hardgrave's time was spent working with the IPAD group on questions concerning data management.

David D. Loendorf, a Civil Service employee of the Army Air Mobility Research and Development Laboratory and assigned to the Structures and Dynamics Division, has been contributing to the ICASE Prime 300 minicomputer project. He is studying the feasibility and methodology of using

mini-computers to handle the computer-graphics aspects of aircraft design and to look at the interfacing of graphics application programs with a data base. In particular, he will implement three computer programs. The first will be a graphics software package (CKLIB) developed at the University of Michigan. The second will be a finite element program (SNAP) developed by Lockheed, and the third will be a fuselage design package (FADES) developed at Langley Research Center. It is planned that these three packages will be merged into one program which will use interactive graphics to aid the design engineer in making decisions and guiding the design process. This work should also give insight into how much of the design process can be handled using mini-computers and how efficient it will be if the mini-computer is time-shared with another activity such as data-base management.

Ms. M. Castano and Mr. R. Murphy are providing programming support for much of the work on the Prime 300.

Prof. James C. Browne of The University of Texas spent the period June 1 - July 19, 1974 at ICASE followed by two shorter visits.

Prof. Browne's primary activity during this period was with the ACD Computer Integration Study Group. This study group, consisting of R. Hofler, D. Booth, D. Eckert, J. Harris, and Prof. Browne, had as its goal development of a long-range plan for the integration of current and future computer facilities. The roles played by Dr. Browne in this study group included: (1) a survey of computer users both within and outside ACD (13 users, representing most of the large computer system users, were interviewed); (2) preparation of a number of working papers relating to the establishment of a store and forward network configuration and for

modeling and simulation of the network; (3) preparation of recommendations for improvement of the current ICOPS operating system. The study group made a number of presentations, accompanied by written summaries, to ACD members. Dr. Browne also participated in a number of meetings with various ACD personnel during the course of the study, as well as consulting with members of other Langley projects.

Prof. Forest Baskett of Stanford University spent the period July 1 - 19, 1974 at ICASE. He studied various aspects of the ICOPS operating system and made certain recommendations to ACD for improving the turnaround service by adding express queues. He also consulted with Drs. Browne and Sherman on various questions concerning the modeling and simulation of the computer complex, and with Drs. Knight and Sherman on paging system performance using the virtual memory of the Prime 300.

Mr. Thomas Wright, of the National Center for Atmospheric Research, spent the period August 5 - 16, 1974 implementing the NCAR computer graphics system on the CDC 6000's at ACD and also partially on the Prime 300. This system has a number of sophistocated routines, especially for contouring, and should be a useful addition to the ACD library. During his short stay, Mr. Wright also consulted with a number of Langley people on the use of the NCAR routines and on other applications of computer graphics.

# 2. Other ICASE Activities

Preparations continued for the Second Langley Conference on Scientific Computing to be held in Virginia Beach, Virginia on October 21 and 22, 1974. The meeting is cosponsored by ICASE and the Society for Industrial and Applied Mathematics (SIAM) and will have three invited lecturers, a panel discussion, and over thirty contributed papers on the theme Numerical Methods for Parallel and Vector Processors.

Several ICASE people were active with the local universities and the professional societies. Dr. Gunzburger taught a graduate course on Mathematical Techniques in Fluid Dynamics at William and Mary College in the Spring, 1974 semester. Dr. Ortega continued as coadvisor (with Prof. Bruce Chartres) of the PhD dissertation of Mr. J. J. Lambiotte of ACD at the University of Virginia. Dr. Cline continued as coeditor of the Algorithms Department of the Communications of the Association of Computing Machinery (ACM) and was appointed as Associate Editor of the new ACM Transactions on Mathematical Software. Dr. Ortega participated in a three-day meeting of the Curriculum Committee on Computer Science of the ACM for the purpose of updating the 1968 recommendations (Curriculum '68) on undergraduate and graduate programs in Computer Science. He also continued on the Program Committee of SIAM.

Almost all ICASE members consulted with various Langley personnel in addition to the collaborative research described in the previous section. For example, Dr. Cline worked with Dr. E. Armstrong of FDCD on solutions to the matrix equation X = AXB+C; with Prof. A. Noor of GWU on the effect of Cholesky factorization on the conditioning of the reduced submatrices; and with Dr. Stephen Park of ACD on contour mapping of rectangular arrays of data. Dr. Poole consulted with Charles Fox of HSAD on the best ways to solve linear equations with dense 1000 x 1000 coefficient matrices, and with Prof. Charles Cooke of ODU on the possible use of profile reduction and decomposition algorithms. Dr. Rosenbaum also worked with Dr. Armstrong on two-point boundary value problems with discontinuities in the right hand side, and with George Haigler of ACD on testing some ordinary differential equation subroutines for possible inclusion in the ACD subroutine

library. Prof. Gustafsson discussed various aspects of atmospheric and oceanic circulation models with Dr. Hugh Davies and Richard Turner of SATD. Dr. Terry Hardgrave spent a sizeable portion of his time working with the IPAD group of SDD on various aspects of data management. Profs. James Browne and Stephen Sherman had a series of meetings with Drs. Roland Bowles and Terry Straeter of ACD on the TCV project and related problems.

ICASE participated in forming a "Computer Graphics Group" for the purpose of sharing information on current graphics activities and capabilities at Langley as well as increasing our general level of graphics expertise. The group consisted of about 15 NASA, ICASE, and GWU people and met regularly throughout the summer. A primary focus of the Group was a series of lectures by Prof. Hussein Kamel of the University of Arizona who was visiting Langley for the summer. These were supplemented by David Loendorf of SDD and Robert Smith of ACD as well as by several visiting lecturers. The summer's activity was completed by a two-day meeting and review with Profs. Richard Phillips of the University of Michigan and Victor Wallace of the University of North Carolina.

### APPENDIX A. ICASE STAFF

March 1, 1974 - August 31, 1974

### I Administrative

James M. Ortega, Director Ph.D., Mathematics, Stanford University, 1962 Numerical analysis

Robert G. Voigt, Assistant Director Ph.D., Mathematics, University of Maryland, 1969 Numerical analysis

John C. Tredennick, Executive Assistant (Until May 31, 1974)

Charlotte E. Bristow, Secretary (June 1 - August 9, 1974)

Linda T. Johnson, Secretary, (Part-time since May 1, 1974)

Margaret H. Mann, Secretary, (Since May 1, 1974)

Myrtle H. Wells, Secretary (Until June 7, 1974)

### II Advisory Committee

Bruce W. Arden, Professor and Chairman of Computer Science and Electrical Engineering, Princeton University.

Samuel D. Conte, Professor and Chairman of Computer Science, Purdue University

Eugene Isaacson, Professor of Mathematics, Courant Institute, New York University

Randal M. Robertson, Dean, Research Division, Virginia Polytechnic Institute and State University

# III Term Appointments

Alan K. Cline - Ph.D., Mathematics, University of Michigan, 1970. Computational linear algebra and approximation theory. Joined ICASE September, 1973. Current appointment runs to September 1975.

Max D. Gunzburger - Ph.D., Mathematics, New York University, 1969. Fluid dynamics and numerical solution of partial differential equations. Joined ICASE September 1973. Current appointment runs to September 1975.

W. Terry Hardgrave - Ph.D., Computer Science, University of Texas at Austin, 1972. Data management and operating systems. Joined ICASE in January 1974. Current appointment runs to September 1975.

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Virginia S. Jordan - Ph.D. Candidate, Applied Mathematics, Harvard University. Differential equations and fluid dynamics. At ICASE September 1973 - June 1, 1974 on part-time appointment.

Richard C. Raffenett: - Ph.D., Physical Chemistry, Iowa State University, 1971. Computational chemistry - Joined ICASE in March 1974. Current appointment runs to March 1975.

Jerrold S. Rosenbaum - Sc.D., Applied Mathematics, Columbia University, 1971. Numerical solution of ordinary differential equations. Joined ICASE August 1973. Current appointment runs to June 1975.

### IV Visiting Scientists

A. Kadir Aziz - Ph.D., Mathematics, University of Maryland, 1958. Professor of Mathematics at the University of Maryland at Catonsville. Nonlinear partial differential equations and finite element methods for gas dynamics problems. At ICASE from September 1, 1973 to June 1, 1974.

A. Jerry Baker - Ph.D., Engineering Science, SUNY-Buffalo, 1970. Principal Scientist, Bell Aerospace Company. Computational fluid dynamics. At ICASE July 8-19, 1974.

Victor B. Basili - Ph.D., Computer Sciences, University of Texas at Austin, 1970. Assistant Professor of Computer Science, University of Maryland. Programming languages and compiler construction. At ICASE June 3-7, July 1-2, 1974.

Forest Baskett - Ph.D., Computer Science, University of Texas at Austin, 1970. Assistant Professor of Electrical Engineering and Computer Science, Stanford University. Operating systems and computer architecture. At ICASE July 1-19, 1974.

James C. Browne - Ph.D., Physics, University of Texas at Austin, 1960, Professor and Chairman of Computer Science and Professor of Physics at the University of Texas at Austin. Operating Systems. At ICASE June 1 - August 1, 1974.

George J. Fix - Ph.D., Mathematics, Harvard University, 1968. Associate Professor of Mathematics at the University of Michigan. Numerical methods for partial differential equations and, in particular, finite element methods for fluid dynamics. At ICASE May 15 - August 21, 1974.

Alan George - Ph.D., Computer Science, Stanford University, 1971. Associate Professor of Computer Science, University of Waterloo. Numerical linear algebra and finite element methods. At ICASE May 1 - August 1, 1974.

C. William Gear - Ph.D., Mathematics, University of Illinois, 1960. Professor of Computer Science and Applied Mathematics, University of Illinois. Numerical solution of ordinary differential equations. At ICASE June 17-28, 1974.

Michael Ghil - M.S., Mathematics, New York University, Research Associate at Courant Institute. Numerical simulation of atmospheric and oceanic circulation. At ICASE August 1-30, 1974.

Gene H. Golub - Ph.D., Mathematics, University of Illinois, 1959. Professor of Computer Science at Stanford University. Large-scale matrix problems and numerical solution of partial differential equations. At ICASE August 26-28, 1974.

David Gottlieb - Ph.D., Numerical Analysis, Tel Aviv University, 1972. Visiting Professor of Applied Mathematics, Massachusetts Institute of Technology. Numerical solution of hyperbolic equations. At ICASE June 1 - August 31, 1974.

Bertil Gustafsson - Ph.D., University of Uppsala (Sweden), 1968. Acting Professor of Computer Science, University of Uppsala. Numerical solution of partial differential equations. At ICASE July 1, 1974 - June 30, 1975.

Moshe Israeli - Ph.D., Applied Mathematics, Massachusetts Institute of Technology, 1971. Senior Lecturer, Applied Mathematics, The Technion, Israel. Computational fluid dynamics. At ICASE July 29 - August 2, 1974.

John C. Knight - Ph.D., Computer Science, University of Newcastle-upon-Tyne, 1973. Assistant Professor of Computer Science at the University of West Virginia. Virtual and paged memories. At ICASE May 15 - August 1, 1974.

Heinz-Otto Kreiss, Ph.D., Mathematics, Royal Institute of Technology (Stockholm) 1961. Professor of Computer Science, University of Uppsala (Sweden). Numerical solution of hyperbolic equations. At ICASE April 5 and August 29-30, 1974.

Jorge J. More - Ph.D., Mathematics, University of Maryland, 1970. Assistant Professor of Computer Science at Cornell University. Numerical analysis and optimization. At ICASE June 1 - August 1, 1974.

Joseph Oliger, Ph.D., Computer Science, University of Uppsala, 1973. Staff scientist at NCAR and Assistant Professor of Computer Science at Stanford University. Numerical solution of hyperbolic equations. At ICASE August 12-16, 1974

Steven Orszag - Ph.D., Physics, Princeton University, 1966. Associate Professor of Applied Mathematics, Massachusetts Institute of Technology, Computational fluid dynamics. At ICASE July 29 - August 2, 1974.

William G. Foole, Jr. - Ph.D., Computer Science, University of California at Berkeley, 1970. Assistant Professor of Mathematics at the College of William and Mary. Development of algorithms for vector processors. At ICASE from September 1, 1973 to June 1, 1974 and then half-time through June 1975.

Gerard R. Richter - Ph.D., Applied Mathematics, Harvard University, 1971. Assistant Professor of Mathematics, University of Michigan. Numerical solution of integral equations. At ICASE June 1 - August 1, 1974.

Stephen W. Sherman - Ph.D., Computer Science, University of Texas at Austin, 1972. Assistant Professor of Computer Science at the University of Houston. Operating systems. At ICASE March 8-11, 1974 and May 6, 1974 - September 1, 1975.

Harold S. Stone - Ph.D., Electrical Engineering, University of California, Berkeley, 1963, Associate Professor of Computer Science and Electrical Engineering, Stanford University. Parallel processing. At ICASE May 13-17, 1974.

Micha Wolfshtein - Ph.D., Mechanical Engineering, University of London, 1968, Senior Lecturer. Aeronautical Engineering, The Technion, Israel. Computational fluid dynamics. At ICASE August 18, 1974 - August 18, 1975.

Thomas Wright - B.S., Applied Mathematics, University of Colorado, 1970. Staff Programmer. NCAR. Computer graphics. At ICASE, August 5-16, 1974.

David H. Y. Yen - Ph.D., Mathematics, New York University, 1965. Professor of Mathematics, Michigan State University. Engineering mechanics. At ICASE January 1 - June 30, 1974.

### V Affiliated. Langley Members

John C. Knight (See description under Visiting Scientists) Analysis and Computations Division, Langley Research Center.

David D. Loendorf - M.S., Structural Engineering, Old Dominion University, 1970. Application of computer graphics to structural engineering. Assigned to the Structures and Dynamics Division of Langley Research Center by the Army Air Mobility Research and Development Laboratory.

# VI Student Assistants

Ron Boisvert, Graduate student at William and Mary College. Numerical analysis. At ICASE from August 19, 1974 as half-time programming assistant.

Marjorie Castano - Undergraduate at Christopher Newport College. Half-time programming assistant since June 17, 1974.

Martin R. Cordes - M.S., Information and Computer Science, University of California - San Diego, 1972. Numerical Analysis. At ICASE June 15 - Sept. 15, 1974.

Don E. Heller - Graduate student in Computer Science at Carnegie-Mellon University, Ph.D. expected 1975. Numerical methods for parallel processors. At ICASE May 20 - August 23, 1974.

Dennis Jespersen - Graduate student in Mathematics at University of Michigan. Ph.D. expected 1975. Numerical solution of partial differential equations. At ICASE July 11 - August 31, 1974.

Susan M. McCabe - B.S., Mathematics, College of William and Mary, 1973. Graduate student at William and Mary. At ICASE September 1, 1973 - August 30, 1974 as half-time programming assistant.

# APPENDIX B. REPORTS AND PUBLICATIONS

March 1, 1974 - August 31, 1974

1. Alan K. Cline and J. F. Walsh: A Regression Analysis Subroutine Package. ICASE, April 19, 1974, 24 pages. Submitted to the ACM Transactions on Mathematical Software.

- 2. Max D. Gunzburger, C. H. Liu, Lucio Maestrello, and Lu Ting: Sound Propogation through a Real Jet Flow Field with Scattering due to Interaction with Turbulence. ICASE, May 13, 1974, 14 pages. AIAA Preprint No. 74551. Submitted to the AIAA Journal.
- 3. Don E. Heller: On the Efficient Computation of Recurrence Relations. ICASE, June 13, 1974, 4 pages. Submitted to the IEEE Transactions on Computers.
- 4. Jules J. Lambiotte, Jr. and Robert G. Voigt: The Solution of Tridiagonal Linear Systems on the CDC STAR-100 Computer. ICASE, July 19, 1974, 48 pages. Submitted to the ACM Transactions on Mathematical Software.
- 5. Norman E. Gibbs, William G. Poole, Jr., and Paul K. Stockmeyer: An Algorithm for Reducing the Bandwidth and Profile of a Sparse Matrix. ICASE, July 22, 1974, 30 pages. Submitted to the SIAM Journal on Numerical Analysis.
- 6. Alan George: A Negative Result on Sparse Matrix Splitting in the Context of Gaussian Elimination. ICASE, July 25, 1974, 16 pages. Submitted to the SIAM Journal on Numerical Analysis.
- 7. Jerrold S. Rosenbaum: Conservation Properties of Numerical Integration Methods for Systems of Ordinary Differential Equation. ICASE, August 15, 1974, 9 pages. Submitted to the Journal of Computational Physics.
- 8. William G. Poole, Jr. and Robert G. Voigt: Numerical Algorithms for Parallel and Vector Computers: An Annotated Bibliography, ICASE, August 19, 1974, 44 pages. Submitted to Computing Reviews.
- 9. A. Kadir Aziz: On Numerical Solution of Equations of Elliptic-Hyperbolic Type, ICASE, August 20, 1974, 15 pages. Submitted to Mathematics of Computation.
- 10. Don E. Heller: Some Aspects of the Cyclic Reduction Algorithm for Block Tridiagonal Linear Systems, ICASE, August 22, 1974, 22 pages. To be submitted to the SIAM Journal on Numerical Analysis.
- 11. Alan K. Cline: A Descent Method for the Uniform Solution of Over-Determined Systems of Linear Equations. ICASE, August 23, 1974, 31 pages. To be submitted to the SIAM Journal on Numerical Analysis.
- 12. D. O. Swint and David H. Y. Yen: Periodic Solutions in a Class of Non-linear Dual-Mass Systems, ICASE, August 30, 1974, 19 pages. To appear in the Proceedings of the First International Symposium on Computational Methods in Nonlinear Mechanics.

A PLAN

# APPENDIX C. ICASE SEMINAR PROGRAM

March 1, 1974 - August 30, 1974

March 5	Prof. Richard S. Varga, Department of Mathematics, Kent State University: "Heat Conduction Problems and Approximation Theory"
March 15	Prof. Werner C. Rheinboldt, Department of Computer Science and Mathematics, University of Maryland: "The Solution of Large Sparse Matrix Problems Based on an Arc-Graph Structure"
March 26	Professor Eugene Isaacson, Courant Institute of Mathematical Sciences, New York University: "Mountain Winds Revisited"
April 5	Prof. Heinz-Otto Kreiss, University of Uppsala (Sweden) and University of Wisconsin: "Finite Difference vs. Finite Element Methods"
April 16	Dr. Robert G. Voigt, ICASE: "On Solving Tridiagonal Linear Systems on the STAR"
April 25	Prof. W. Morven Gentleman, Computer Science Department, University of Waterloo, Canada: "Applications of Symbolic Computation in Numerical Analysis"
April 29	Dr. Alan K. Cline, ICASE: "A Descent Method for the Uniform Solution to Over-Determined Systems of Linear Equations"
May 3	Prof. William G. Poole, ICASE and College of William and Mary: "An Algorithm for Matrix Bandwidth Reduction"
May 15	Prof. Harold Stone, Department of Computer Science and Electrical Engineering, Stanford University: "Dynamic Memories with Enhanced Random and Sequential Access"
May 16	Prof. Sigram Schindler, Technical University of Berlin: "Generalized Deadlock Prevention in Operating Systems"
May 20	<u>Prof. Andries van Dam</u> , Department of Computer Science, Brown University: "Micro Programmed Intelligent Satellites for Computer Graphics"
May 21	Dr. Henry Merryweather, The Computer-Aided Design Institute, Cambridge, England: "Mini-computers and Graphics"
June 3	Prof. Victor Basili, Department of Computer Science, University of Maryland: "The SIMPL Family of Languages and Compilers"

Dr. Ernst Schrem, Institute for Statics and Dynamics of June 17 Aerospace Structures, University of Stuttgart, Germany: "Some Aspects of the Design of a Programming System for Finite Element Analysis" Dr. Ernst Schrem: "Observations on the Use of Structured Pro-June 18 gramming and Other Modern Software Development Methods" Dr. Thomas I. Boardman, Computer Aided Design Laboratory, June 19 University of Michigan: "Interactive Graphics Communications Systems" Prof. C. William Gear, Department of Computer Science, University June 20 of Illinois: "Error Control in the Integration of Ordinary Differential Equations" Prof. Jack Schwartz, Courant Institute of Mathematical Sciences: June 24 New York University: "Structure of Programming Languages" June 27 Dr. Bengt Lindberg, Department of Computer Science, University of Toronto: "Characterization of Optimal Stepsize Sequences for Methods for Stiff Differential Equations" Prof. Forest Baskett, Department of Computer Science, Stanford July 2 University: "A Survey of Recent Results on Queueing Models of Multiprocessor Systems" <u>Prof. Gerard R. Richter</u>, Department of Mathematics, University of Michigan and ICASE: "Numerical Solution of Fredholm Integral July 10 Equations of the First Kind" Prof. Achi Brandt, Department of Mathematics, Weizmann Institute: July 15 "Fast Numerical Solution of Boundary Value Problems" Prof. David M. Young, Center for Numerical Analysis, University July 17 of Texas at Austin: "On the Surveillance and Acceleration of Iterative Methods for Solving Large Linear Systems" Prof. Alan George, Department of Computer Science, University July 18 of Waterloo and ICASE: "A Negative Result on Sparse Matrix Splitting in the Content of Gaussian Elimination" Prof. James Bunch, Department of Computer Science, Cornell July 22 University: "Symmetric Gaussian Elimination" Dr. Moshe Israeli, Department of Applied Mathematics, Massachusetts July 29 Institute of Technology and the Technion: "A Fourth Order Scheme for a Two-Level Ocean" Mr. Michael Ghil, Courant Institute of Mathematical Sciences, August 2 New York University: "Atmospheric Simulation"

Dr. Willard Miranker, IBM: "Parallel Root-finding"

August 5

- August 9 Prof. Bertil Gustafsson, University of Uppsala and ICASE: "On the Choice of Boundary Conditions for Difference Approximations to Hyperbolic Equations"
- August 13 Prof. Joseph Oliger, National Center of Atmospheric Research and Stanford University: "Initial Boundary Value Problems for Geophysical Fluids"
- August 19 Prof. Richard Phillips, Department of Aerospace Engineering and the Computation Center, University of Michigan: "Use of Interactive Graphics in Interrogation of Large Data Bases"
- August 19 Prof. Victor Wallace, Department of Computer Science, University of North Carolina: "Graphics Languages and the Configuration of Satellite Graphics"
- August 21 Mr. Charles T. Zahn, Stanford Linear Accelerator Center:
  "Implementation of a Structured Language Using the Mortran Macroprocessor"
- August 26 Prof. Gene H. Golub, Department of Computer Science, Stanford University: Solution of Sparse Systems of Linear Equations"

# ICASE

# SEMI-ÂNNUAL REPORT

September 1, 1974 - February 28, 1975

INSTITUTE FOR COMPUTER APPLICATIONS

IN SCIENCE AND ENGINEERING

Operated by the

UNIVERSITIES SPACE RESEARCH ASSOCIATION

at

NASA's LANGLEY RESEARCH CENTER
Hampton, Virginia

### 1. Introduction

ICASE was formed in 1972 under an agreement between NASA's Langley Research Center and the Universities Space Research Association, a consortium of some fifty major universities across the country.

The primary objective of ICASE is to perform research in applied mathematics, numerical analysis, and applied computer science with particular emphasis on application areas of interest to the Langley Research Center. The mechanism of performing such research is through visiting appointments of leading university researchers in these fields, postdoctoral fellowships, and term appointments of younger scientists with no other affiliation. Such appointees, whose training is primarily in mathematics and computer science, are encouraged to work in close collaboration with NASA scientists and engineers on problems of mutual interest. It is hoped that such collaborations will contribute to the continued vitality of applied mathematics and computer science while at the same time make an immediate impact on problems of concern to NASA.

The overall research program of ICASE is directed toward the general area of scientific computing with particular emphasis on bridging the many gaps between theory and practice, and between mathematicians and computer scientists on the one hand and engineers and natural scientists on the other. The major categories of the current ICASE research program are:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR-100.
- b. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
- c. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.
- d. Computer systems and software, with particular emphasis on mini-computers, distributed computing, and computer graphics.

The work in each of these areas will be described briefly in the next section, while other activities are discussed in Section 3.

### 2. The ICASE Research Program

### a. Efficient Use of Vector and Parallel Computers

The major effort in this area centered around the FESS project, a cooperative effort with representatives from the Structures and Dynamics Division, Analysis and Computation Division (ACD), George Washington University (GWU), and ICASE, with the goal of producing a finite element program for STAR. Dr. James M. Ortega, Director of ICASE, has assisted Prof. Ahmed Noor in directing the effort while Dr. Robert G. Voigt, Assistant Director of ICASE, and Prof. William G. Poole, on leave half-time from William and Mary College from September 1, 1974 to June 1, 1975, have taken an active roll in the study of algorithms for the linear systems arising from finite element analysis. After carefully investigating the impact of the STAR on the implementation of several appropriate algorithms with Mr. J. Lambiotte of ACD, specifications have been written for the coding of all the modules necessary for solving the linear systems. The specifications were developed using many of the ideas popularized by the proponents of structured programming; thus the project will provide some insight into the gains and costs of this approach to the development of a large-scale scientific program.

Drs. Poole and Voigt are also working on two projects which should have impact on the FESS program. The first of these is a study of the problem of balancing I/O rate with computation rate on vector computers, and is being carried out in collaboration with Dr. John Knight of ACD. Although the project was motivated by the STAR, the analysis has been parameterized so that it is applicable to a wide class of vector computers, with a variety of peripheral devices; for example, the study permits an analysis of the Texas Instruments ASC. A detailed

analysis is being done for the solution of banded systems of linear equations so large that the problem can not be contained in core.

The other effort of Drs. Poole and Voigt is centered around investigating various solution techniques for the large sparse linear systems arising in finite element analysis. In particular the approach known as substructuring (or dissection) is being investigated with particular emphasis on how the STAR effects these techniques. For example, in general as the number of substructures increases the operation count decreases; however, the vector lengths of the associated arithmetic operations also decrease so that the operations become less efficient for the STAR. Consequently, from the standpoint of timing, there is an optimal number of substructures and this can be predicted based on the work in progress. It is expected that the algorithms chosen will have an impact on the FESS project particularly where the problems are so large they can no longer be contained in core memory. Prof. J. Alan George of The University of Waterloo has served as a consultant on the project.

Dr: Knight continued his collaboration with Prof. Victor Basili of the University of Maryland on the design of a new high-level programming language for the STAR-100. This project was started during the summer of 1974 while Dr. Knight was at ICASE and was discussed briefly in the previous semi-annual report; it has been carried on since then under the auspices of ACD's STAR Project Office and through several visits by Prof. Basili to ICASE. The language, known as SL/1, has been designed to enable the user of the STAR-100 to write efficient programs and to have access to the machine's unique hardware facilities. As such it provides vectors as a basic data type and many vector operators which take advantage of the high level machine instructions. A preliminary report on the design goals has appeared as an ICASE Report and will be

presented by Drs. Basili and Knight at a forthcoming conference on "Programming Languages and Compilers for Parallel and Vector Machines" sponsored by ACM and NASA-Goddard. Continued development by the STAR Project Office has led to a formal definition of the language together with plans for a suitable compiler. This implementation will run on 6000 series machines but produce STAR-100 object programs. Doug Dunlop, a student assistant at ICASE, is assisting Dr. Knight in this implementation.

Prof. Harold S. Stone, of the University of Massachusetts, spent the week of January 6, 1975 at ICASE working on sorting algorithms for the STAR. He compared timings of three algorithms: Quick Sort; a vector version of Quick Sort; and a vector version of Batcher's algorithm with the conclusion that the vector version of Quick Sort was fastest for less than 5000 items. For over 5000 items, vector versions of either Quick Sort or Batcher's algorithm could the fastest depending on the specific number of items. Above 500,000 items Batcher's algorithm was shown to be superior. This work will appear as an ICASE report.

# b. <u>Numerical Analysis</u>

Dr. Poole, in collaboration with Professors N. E. Gibbs and P. K. Stockmeyer of William and Mary, has continued his work in the area of bandwidth and profile reduction algorithms for large sparse matrices. A comprehensive evaluation and comparison study of several reduction algorithms has been completed and has appeared as an ICASE report. The paper has been submitted to the ACM Transactions on Mathematical Software. The primary conclusion was that the algorithm earlier developed by the investigators (ICASE Report, July 22, 1974) was clearly the fastest, usually produced the smallest bandwidth, and along with the King algorithm, was the best profile reducer. However, several inconsistencies concerning the King algorithm were pointed out. Profs. Gibbs, Poole, and

Stockmeyer are currently investigating several variations of that method with the goal of a complete analysis of the algorithm.

Dr. Alan K. Cline, who is at ICASE on a term appointment until September 1975, continued his investigation of the Lanczos and conjugate gradient methods for the numerical solution of large systems of linear equations. A new approach was taken to the analysis of these and related algorithms. The approximate solution is considered as a polynomial in the coefficient matrix applied to the right hand side of the equations, where the polynomial may be selected to minimize various norms and the theory of orthogonal polynomials exploited to yield three term recurrence relations. Of course the resulting algorithms do not change, only the derivation and manner of analyzing them. The convergence theory is easy to develop from this polynomial approach and Dr. Cline has extended the ideas of Kaniel to symmetric indefinite, and non-symmetric problems. Many tests on the algorithm, including ones showing the sharpness of the theoretical convergence bounds, have been carried out. The polynomial approach and the new proofs have also led to the observation that the minimum residal conjugate gradient algorithm (one occasionally discussed but seldom implemented) is applicable to indefinite symmetric systems and thus can handle non-symmetric coefficient matrices by doubling the size of the system. Preliminary presentations of this study were given by Dr. Cline at the Second Langley Conference on Scientific Computing and at the Gatlinburg VI Conference in Germany. Work still to be done includes a detailed error analysis of the methods.

Dr. Cline also continued his work on the NATS project with additional testing of the latest EISPACK codes (a package of subroutines for matrix eigenvalue calculation). In connection with Mr. Ron Boisvert, a student assistant at ICASE, he also considered the adaptation of his previous descent algorithm for overdetermined linear systems (ICASE Report, August 23, 1974) to nonlinear systems of equations.

Prof. Bertil Gustafsson, who is at ICASE for the year July 1, 1974-July 1, 1975 on leave from the University of Uppsala (Sweden), collaborated with Prof. David Gottlieb of the Massachusetts Institute of Technology on a generalization of Du Fort-Frankel type methods for parabolic partial differential equations. The classical second order Du Fort-Frankel difference scheme was generalized to arbitrarily high order accuracy in space for parabolic systems of arbitrary order and in any number of space dimensions. Instead of difference methods, spectral methods or finite element methods can also be used for the spatial part of the differential operator. The schemes are explicit and unconditional stability for the pure initial value problem has been proved under only the condition that the Fourier transform of the principal part has real eigenvalues. Stability for the mixed initial boundary value problem has also been proved for two different fourth order accurate spatial approximations. This work has appeared in an ICASE report which will be submitted to the SIAM Journal on Numerical Analysis and will be presented in an ICASE seminar as well as at the 1975 SIAM National Meeting in June.

The above methods are being applied to a two dimensional flow problem in a domain with an incoming transonic jet in conjunction with the Fluid Mechanics Branch of the High Speed Aerodynamics Division; the mathematical model here is a modified version of the Navier- Stokes equations. To gain insight into the behavior of the solutions, the second order Du Fort-Frankel scheme was programmed first and several numerical experiments made. To be able to handle high Reynolds numbers, a dissipative version of the leap frog scheme was used for the hyperbolic part. Steady-state solutions for the model problem being treated have been compared with solutions which can also be obtained accurately by solving the boundary layer equations and comparison between the two approaches has been very good. The higher order Du Fort-Frankel schemes are now being programmed and numerical experiments on this problem will continue.

Drs. Gottlieb and Gustafsson have also been working with members of the Fluid Mechanics Branch on analyzing some existing codes, in particular, an ADI type method and a modified version of the Hopscotch scheme, for the same model problem. Based on an analysis of the one-dimensional equations, boundary conditions were chosen such that accurate steady-state solutions could be obtained. A point of interest on this problem is that when extrapolation methods were used for all variables at the subsonic downstream boundary, where one of the variables should in fact be prescribed, the Hopscotch method converged to a steady-state solution although it was not correct in the subsonic-transonic region.

Dr. Gustafsson has also pursued two other projects. The first is the problem of calculating the flow about axisymmetric blunt bodies at hypersonic speeds which is of interest to the Advanced Entry Analysis Branch and which was discussed in more detail in the previous semi-annual report. A dissipative difference scheme of the ADI box-type has been defined for the time-dependent equations. The scheme is implicit and a Newton method is used to solve the non-linear algebraic equations. A program has been written by Ron Boisvert and is now being debugged. The second project involves the study of parabolic systems of incomplete type, that is, the Fourier transform of the principal part is not positive definite. The compressible viscous Navier-Stokes equations are of this category. Dr. Gustafsson is studying the well-posedness of such systems for the initial boudnary value problem and preliminary results have been obtained. For the one-dimensional Navier-Stokes equations, well-posed boundary conditions have been derived which go over into well-posed conditions for the hyperbolic part of the system as the Reynolds number tends to infinity.

Prof. Roland Sweet of the University of Colorado spent the week of February 24 at ICASE implementing a package of fast poisson solvers on the CDC 6000's. This set of subroutines was developed at the National Center for Atmospheric Research by Dr. Sweet and Dr. Paul Swarztauber and is based on the cyclic reduction algorithm. Dr. Sweet gave a series of three lectures on the theory and use of this package.

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### c. Computational Research in Science and Engineering

Dr. Jerrold S. Rosenbaum, who is at ICASE on a half-time appointment, has continued his collaboration with Dr. Roland Bowles of ACD and Prof. C. William Gear of the University of Illinois on numerical methods for real time simulation. Further progress has been made in identifying suitable integration methods for various parts of the problem, and a program has been written to display simultaneously magnitude and phase shift errors for methods that are exact for complex eigenvalue pairs. Prof. L. Brown of the University of Virginia also is participating in this project.

Work on special methods for quasilinear systems of ordinary differential equations, developed by Dr. Rosenbaum earlier, has been continued. Special emphasis is on applications to parts of the real time simulation problem. Also, Prof. Gear's suggestion of finding faster approximations to trigonometric functions has been undertaken. Several approximations with an accuracy of only 6 digits have been programmed (both in FORTRAN and COMPASS) and average savings of up to 30% over the standard library programs have been observed. The programs are presently awaiting testing in the actual simulation program.

Prof. George Fix of the University of Michigan completed an ICASE report entitled Finite Elements and Fluid Dynamics which summarized some of the work he had previously done, partly at ICASE, and also gave some directions for future research. This was presented as an invited talk at the First International Symposium on Computational Methods in Nonlinear Mechanics and will appear in the Proceedings of that symposium. A modified version was also given as an invited talk at the 1974 Fall SIAM meeting.

Dr. Max Gunzburger, who is on a term appointment at ICASE until September, 1976, continued his collaboration with Prof. Fix on a study of various boundary conditions that can be imposed on the outflow region in viscous fluid flow problems. The linearized Burger's equation is used as a simple model for both numerical experiments and theoretical study. Comparison is made between the most obvious outflow conditions, e.g. specifying a vanishing function value or a vanishing second derivative at the outflow, and a new integral condition which approximates the mass in the region at any given time. Both the experimental and theoretical results show that all three conditions cause a boundary layer of thickness proportional to the inverse of the Reynolds number to be built up near the outflow. This boundary layer "contains" any errors made in specifying the outflow condition. In the case of integral conditions, the boundary contains the error in the mass, i.e. the difference in the true mass and the approximate mass. This work is now nearing completion.

In collaboration with Prof. L. Ting of the Courant Institute and Dr. C. H. Liu and Mr. Lucio Maestrello of the Acoustics and Noise Reduction Division (ANRD), Dr. Gunzburger has been studying the simulation of the pressure field near a jet by the shedding of vortex rings from the jet exit. If this near-field pressure can be predicted by such a simple model, it would greatly facilitate calculation of the far field noise due to a jet since it would no longer be necessary to compute the turbulent sources of noise within the jet. Some empirical data supplied by Mr. Maestrello is used to determine some of the parameters in the model. A computer program has been written and results show good qualitative agreement with experimental data. This work has resulted in an ICASE report, and is to be presented at the AIAA

Second Aeroacoustics Specialists Conference at Langley in March. Continued refinements of the model are presently being undertaken.

Dr. Gunzburger has continued work on a large program that computes the propagation of sound through a steady jet. The program is not yet operative, and Dr. Gunzburger has been investigating some basic questions that have arisen from the program's performance. Among these are the applicability of Galerkin's Method to wave problems in infinite domains and the question of whether to map infinite domains to finite domains or to truncate them and impose radiation conditions. This overall project is expected to continue for some time.

Work continued on the development of a code, based on a Galerkin approach using cubic splines, for the modeling of chemical kinetic transport in the atmosphere. This project, which is being done in consultation with Dr. R. Boughner and others of the Space Systems Division (SSD) at Langley, was described in more detail in the previous semi-annual report. Mr. Martin Cordes, who was at ICASE from June until December 1974, was the primary developer of the code with consultation from members of SSD as well as Prof. Fix and Drs. Gunzburger and Rosenbaum of ICASE. At the time of Mr. Cordes' departure from ICASE, there were still difficulties in the code, both in its ability to produce accurate results and in its efficiency relative to finite difference methods. Work on the code is now continuing at the University of Michigan under Prof. Fix's direction with continuing assistance from Mr. Cordes. Dr. Rosenbaum is also modifying the part of the program that integrates a system of stiff ordinary differential equations by a trapezoidal rule in order to make it into a separate package for use on other problems.

Prof. Micha Wolfshtein is at ICASE for a one-year stay while on sabbatical leave from the Technion in Israel. In collaboration with Dr. R. Hirsh and Ms. B. Pitts of the Fluid Mechanics Branch he has been developing a new method for the solution of non-linear parabolic type partial differential equations by an ADI procedure. Although the method is second order accurate in time, it does not require either iterations or predictor-corrector techniques to overcome the non-linearity of the equations; thus the computational effort required for the solution of non-linear problems becomes nearly identical to that required for the linear case. However, the method depends on non-linearities which are formed by products of two functions and/or spatial derivatives. The non-linear convection terms of the Navier-Stokes equations are suitable for such treatment. The method has been tested for a two-dimensional analog of Burger's equation which is similar to the Navier-Stokes equations, and a comparison was made with results obtained from an ADI integration where the nonlinear terms were lagged one time level, producing only first order accuracy in time, as well as with a Jacobi iteration. All the techniques converged to the exact solution. However, the new method is more accurate than the others in the transient region, and allows larger time steps to be used. An ICASE report describing the method and the preliminary tests is now being prepared, and further testing with applications to three dimensional turbulent free shear flows will be carried out.

Dr. Wolfshtein also continued his long term program of the modeling of turbulence based on spectral distribution of the turbulence energy. This work splits into two parts: definition of the model, and solution of the resulting equations. Some existing models have been studied in order to allow a meaningful choice of a final model for the equation of turbulence energy in the wave number space. Some numerical problems associated with such equations were also investigated. It was found that the energy equation is very stiff,

and special techniques will be required to produce a stable solution to it. Work on this project is continuing.

Dr. Richard Raffenetti, who is at ICASE on a term appointment until September 1975, is carrying out computations on an atmospheric pollution problem in conjunction with Dr. Donald Phillips of the Environmental and Space Sciences Division (ESSD). Of interest is a mechanism for the oxidation of nitric oxide(NO) to NO2. Several points on the potential surface of interaction of two diatomics  ${\tt NO}$  and  ${\tt O_2}$  have been evaluated at the Hartree-Fock self-consistent field level in order to check for possible direct mechanisms. For these preliminary studies the geometries of the complex are being restricted by keeping the diatomics coplanar and changing only the inter-diatomic separation and orientation. Most calculations to date are in geometries classified as  $C_{2v}$  (near  $D_{3h}$ with N central) and in a trans chain (with N not at an end). Indications are that the cis chain will also obtain geometries of interest due to their low energies. Some attention is also being given to establishing a best equilibrium geometry for the  ${\rm NO_3}$  complex where all bond distances are relaxed. Preliminary findings were reported at the Southeastern Regional meeting of the American Chemical Society in Norfolk in October.

Dr. Raffenetti is working on a project bearing upon the removal of chlorine from the stratosphere which is being carried out in conjunction with Dr. Philips and with the support of Dr. Gerald Pellett of the Space Applications and Technology Division. They have computed the Hartree-Fock self-consistent field energies of the complex for a dozen geometries to date. Contrary to what was hoped there is an indication that the isolated complex system will be predicted to be no more stable than found by others in some very early calculations. They do find that their improved procedures produce significantly different geometry parameters and therefore certain features of

the potential energy surface are being investigated further. Procedures necessary for the additional configuration mixing or configuration interaction treatment, which will provide higher level data, are being considered.

In conjunction with, Drs. Phillips and Edward Long of ESSD,
Dr. Raffenetti is consulting on a feasibility study of energy production via
production of hydrogen from water using sunlight as the main energy source.
In order that dissociation of water or a water complex may be carried out
utilizing the sun's low energy radiation, it is necessary to study the
potential energy surfaces of the ground and lower excited states of water.
Preliminary investigations are being carried out by Dr. Long. The improved
virtual orbital procedure is being utilized in addition to the Hartree-Fock
self-consistent field method.

# d. Computer Systems and Software

Prof. Stephen Sherman of the University of Houston is spending the period May 1974 to September 1975 at ICASE. Dr. Sherman is principal investigator on a supplementary NASA grant to ICASE which has allowed the acquisition of a PRIME 300 mini-computer system and associated graphics terminals. The system was installed in August 1974, and is being used to study the potentialities of a low-cost mini-computer for interactive graphics, data base management, and a variety of other functions. The mini-computer can be either stand-alone or connected to a larger host computer. This study is being co-sponsored by ACD and by the IPAD project of the Structures and Dynamics Division (SDD).

Dr. Sherman made a study of different scheduling and paging algorithms for the PRIME, and a new job scheduling algorithm was implemented that made a 700% improvement in one test case. The MULTICS paging algorithm, (without the dirty page option) was also tried and gave improvements from 3%

to 11% in various tests. A hardware change has been made in the CPU that will allow use of an algorithm that takes advantage of information on altered (dirty) pages. This CPU change has not been checked out although the microcode to try the new hardware capability is ready. This should allow substantial experimentation with several realistic paging algorithms.

Dr. Sherman also completed an ICASE report on previous research in trace-driven modeling of computer systems. This work was done in collaboration with Drs. J. C. Browne and J. Howard of the University of Texas and was presented at the 1974 ACM meeting as well as at a conference in Germany.

Dr. W. Terry Hardgrave, who is at ICASE on a term appointment until September 1975, is nearing completion of the final report for the supplemental NASA grant (NSG 1068) on set theory applications in information systems. This study concerns the potential of a data management system based on extended set theory, and in particular, the role of such a system in a local computer network with a large mass storage device. Such an approach has a number of possible advantages both for users as well as the central computing facility. As a part of the study, the existing Set-Theoretic Data System (STDS) developed by STIS, Inc. was used by remote access to the Computer Center at Wayne State University. A number of actual data bases from Langley were used and various scenarios compiled documenting the use of this system.

Dr. Hardgrave also continued work on the Macro Processor 3 (MP3)/SGOL development. MP3 is an improved version of the MORTRAN macro processor (MP2) developed at the Stanford Linear Accelerator Laboratory (SLAC) and SGOL is an advanced programming language developed by Charles Zahn at SLAC. This work is important to Langley because of the SL/1 language development for STAR and it is also of possible use in defining an IPAD development language. The set processor being developed for the Prime will be written in SGOL thereby providing a large measure of portability and structured, readable code; its initial design is now almost complete.

Dr. Hardgrave has consulted frequently with the IPAD Development Section of SDD and, as part of this consultation, completed a first draft of a potential report on information system requirements for computer-aided aircraft design.

Dr. Hardgrave developed a high level communication system (VENUS) that provides for general interaction and file transfer between the PRIME mini-computer and a host machine. Together with enhancements to the operating system that have been made by Dr. Sherman, this allows the PRIME to communicate through a coupler to any host machine that has a 110 or 300 baud dial-up facility. So far, communications have been completed with the Langley KRONOS system, the KRONOS system at Boeing in Seattle, MTS at the University of Michigan and Wayne State University, the University of Texas at Austin, and MITLAB via the ARPANET.

Mr. David Loendorf, a Civil Service employee of the Army who is assigned to the Structures and Dynamics Division, continued his work on computer graphics using the ICASE PRIME. The Tektronix graphics subroutine package was modified to handle all the hardware capabilities of the 4014 display unit while still remaining compatible with the 4010-4012 displays. One of the more important capabilities of the 4014 is the write-thru mode, which allows data to be placed on the screen in a refreshed manner. However, at 9600 baud only a few vectors can be displayed without flicker, and therefore this capability does not appear feasible at time-sharing baud rates. However, it is believed that a dedicated CP, in the form of a micro-computer, could handle the refreshing requirements. Preliminary work in this direction has been done with Prof. T. Boardman of the University of Michigan, who will spend the summer of 1975 at ICASE.

Mr. Loendorf has also added a three-dimensional graphics capability which allows rotations, scaling, translations, and perspectives. Graphics application packages have been implemented in the aerodynamics area, and are being

used by NASA engineers. The finite element program SNAP has been implemented and is in daily use by NASA engineers in the structures area. An interactive capability for checking input is currently being implemented for SNAP, and when finished, will give a user the ability to view the discretized model and change incorrect data quickly.

Mr. Loendorf and Dr. Sherman are also developing a prototype data base manager for the PRIME. This program will be used by John Decker of the Space Systems Division and others on an experimental basis before proceeding with a more sophisticated system which will be implemented in cooperation with ACD. Mr. Loendorf will also continue developing the system to be more useful in his own computer graphics research.

All of the work on the mini-computer project has benefited substantially from the programming support of Ms. M. Castano and Mr. R. Murphy, student assistants at ICASE.

# 3. Other ICASE Activities

The Second Langley Conference on Scientific Computing was held in Virginia Beach, VA, on October 21 and 22, 1974. The meeting, which was cosponsored by ICASE and the Society for Industrial and Applied Mathematics (SIAM), was attended by almost 200 people. A description of the meeting, which appeared in SIAM News, is given in Appendix D.

Preparations are continuing for a conference on Applications of Computer Graphics in Engineering to be sponsored by NASA-Langley and cosponsored by ICASE. The meeting will be held at Langley Research Center on October 1 and 2, 1975, and will include about a dozen invited lectures as well as contributed papers. David Loendorf is Coordinator for the conference and Drs. Ortega and Voigt are serving on the Conference Committee.

Preliminary work has begun on the next ICASE Conference on Scientific

Computing. Tentative plans call for the meeting to be held in the Tidewater, Virginia area during the Spring of 1976. The theme will be on the interface between computer science and scientific and engineering calculations.

Several ICASE members have been involved in teaching activities. Dr. Gunzburger is giving a second year graduate course on partial differential equations at George Washington University during the current spring semester while Dr. Wolfshtein is offering an advanced topics course on turbulent flow at Old Dominion University. Dr. Gustafsson taught a two-part short course at ICASE on Stability Theory for Difference Approximations to Time Dependent Partial Differential Equations. Almost 40 people attended Part I of the course while about 12 continued for the more advanced Part II. A third and final part is planned for sometime this Spring. Dr. Ortega gave a two-week short course in Advanced Linear Algebra for which about 60 people signed up. Additional short courses are planned for the coming months. Dr. Ortega also continued as coadvisor (with Prof. Bruce Chartres) of the Ph.D. dissertation of Mr. J. Lambiotte of ACD at the University of Virginia.

In the professional societies, Dr. Cline continued as coeditor of the Algorithms Department of the Communications of the Association of Computing Machinery (ACM) and as Associate Editor of the ACM Transactions on Mathematical Software. Dr. Ortega continued as a member of the Program Committee of SIAM and became a member of a panel sponsored by the National Science Foundation to report on computer science research. This is a two to three year study whose goal is to document the current state of research in all areas of computer science and computer engineering and to make projections of future directions and efforts. The steering committee of the overall study is being chaired by Prof. B. W. Arden, a member of the ICASE Scientific Council.

Almost all ICASE members consulted with various NASA personnel in addition to the collaborative research described in the previous section.

## Appendix A. ICASE Staff

## I. Administrative

James M. Ortega, Director Ph.D., Mathematics, Stanford University, 1962 Numerical Analysis

Robert G. Voigt, Assistant Director Ph.D., Mathematics, University of Maryland, 1969 Numerical Analysis

Margaret H. Mann, Secretary

Linda T. Johnson, Secretary (Part-time)

Barbara K. Porter, Secretary (Part-time)

## II. Scientific Council

Bruce W. Arden, Professor and Chairman of Computer Science and Electrical Engineering, Princeton University.

James C. Browne, Frofessor of Computer Science and of Physics at the University of Texas at Austin.

Samuel D. Conte, Professor and Chairman of Computer Science, Purdue University.

Eugene Isaacson, Professor of Mathematics, Courant Institute, New York University.

Randal M. Robertson, Dean, Research Division, Virginia Polytechnic Institute and State University.

# III. Term Appointments

Alan K. Cline - Ph.D., Mathematics, University of Michigan, 1970. Computational linear algebra and approximation theory. Joined ICASE September 1973. Current appointment runs to September 1975.

Max D. Gunzburger - Ph.D., Mathematics, New York University, 1969. Fluid dynamics and numerical solution of partial differential equations. Joined ICASE September 1973. Current appointment runs to September 1976.

W. Terry Hardgrave - Ph.D., Computer Science, University of Texas at Austin, 1972. Data management and operating systems. Joined ICASE in January 1974. Current appointment runs to September 1975.

- Richard C. Raffenetti Ph.D., Physical Chemistry, Iowa State University, 1971. Computational Quantum Chemistry. Joined ICASE in March 1974. Current appointment runs to September 1975.
- Jerrold S. Rosenbaum Sc.D., Applied Mathematics, Columbia University, 1971. Numerical solution of ordinary differential equations. Joined ICASE August 1973. Current appointment is half-time to June 1975.

# IV. <u>Visiting Scientists and Consultants</u>

Victor B. Basili - Ph.D., Computer Science, University of Texas at Austin, 1970. Assistant Professor of Computer Science, University of Maryland. Programming languages and compiler construction. At ICASE December 18-20 and 30, 1974.

Forest Baskett - Ph.D., Computer Science, University of Texas at Austin, 1970. Assistant Professor of Electrical Engineering and Computer Science, Stanford University. Operating systems and computer architecture. At ICASE November 27-29, 1974.

Thomas L. Boardman - Ph.D., Mechanical Engineering, Purdue University, 1973. Assistant Professor of Industrial Engineering, University of Michigan. Computer graphics and computer-aided design. At ICASE October 15-17, 1974, January 2-8, 1975 and May through August 1975.

- R. Leonard Brown, Ph.D., Computer Science, University of Illinois, 1974. Assistant Professor of Computer Science and Applied Mathematics, University of Virginia. Numerical solution of ordinary differential equations. At ICASE January 6-10, 1975 and May and June 1975.
- Martin R. Cordes M.S., Information and Computer Science, University of California San Diego, 1972. Numerical Analysis. At ICASE June 15 December 13, 1974.
- George J. Fix Ph.D., Mathematics, Harvard University, 1968. Associate Professor of Mathematics at the University of Michigan. Numerical methods for partial differential equations. At ICASE December 16-21, 1974 and June through August 1975.
- J. Alan George Ph.D., Computer Science, Stanford University, 1971. Associate Professor of Computer Science, University of Waterloo. Numerical linear algebra and finite element methods. At ICASE January 31 through February 1, 1975.
- C. William Gear Ph.D., Mathematics, University of Illinois, 1960. Professor of Computer Science and Applied Mathematics, University of Illinois. Numerical solution of ordinary differential equations. At ICASE October 17-18, 1974, January 7-10, 1975 and May and June 1975.
- Gene H. Golub Ph.D., Mathematics, University of Illinois, 1959. Professor of Computer Science at Stanford University. Numerical solution of large-scale matrix problems.

David Gottlieb - Ph.D., Numerical Analysis, Tel Aviv University, 1972. Visiting Professor of Applied Mathematics, Massachusetts Institute of Technology. Numerical solution of hyperbolic equations. At ICASE November 4-5, December 16-19, 1974 and January 6-9, January 19, 1975, and then June 1975-.

Bertil Gustafsson - Ph.D., Computer Science, University of Uppsala (Sweden), 1968. Acting Professor of Computer Science, University of Uppsala. Numerical solution of partial differential equations. At ICASE July 1, 1974 - June 30, 1975.

William G. Poole, Jr., - Ph.D., Computer Science, University of California at Berkeley, 1970. Assistant Professor of Mathmetics at the College of William and Mary. Computational Linear Algebra. At ICASE half-time from September 1, 1974 to June 1, 1975.

Stephen W. Sherman - Ph.D., Computer Science, University of Texas at Austin, 1972. Assistant Professor of Computer Science at the University of Houston. Operating Systems and Mini Computers. At ICASE May 6, 1974 - September 1, 1975.

Harold S. Stone - Ph.D., Electrical Engineering, University of California at Berkeley, 1963, Professor of Computer Science, University of Massachusetts. Parallel processing. At ICASE January 6-10, 1975.

Roland A. Sweet, Ph.D., Mathematics, Purdue University, 1967. Associate Professor of Mathematics at the University of Colorado at Denver. Numerical Solution of Partial Differential Equation. At ICASE February 24-28, 1975.

Micha Wolfshtein - Ph.D., Mechanical Engineering, University of London, 1968, Senior Lecturer, Aeronautical Engineering, The Technion, Israel. Computational Fluid Dynamics. At ICASE August 18, 1974 - August 18, 1975.

# V. Affiliated Langley Member

David D. Loendorf - M. S., Structural Engineering, Old Dominion University, 1970. Application of computer graphics to structural engineering. Assigned to the Structures and Dynamaics Division of Langley Research Center by the Army Air Mobility Research and Development Laboratory.

# VI. Student Assistants

Ronald F. Boisvert - Graduate Student at William and Mary College. Numerical analysis. Half-time programming assistant since August 1974.

Marjorie Castano - Undergraduate at Christopher Newport College. Halftime programming assistant since June 1974.

Douglas Dunlop - Undergraduate at William and Mary College. Half-time programming assistant since January 1975.

Ron Murphy - Undergraduate at Christopher Newport College. Half-time programming assistant since June 1974.

#### Appendix B. ICASE Reports

#### September 1, 1974 - February 28, 1975

- 1. Stephen W. Sherman, John H. Howard, Jr. and James C. Browne: Trace Driven Studies of Deadlock Control and Job Scheduling. ICASE, September 23, 1974, 18 pages. To appear in Springer-Verlag Lecture Notes in Computer Science.
- 2. W. Terry Hardgrave: Positional Versus Keyword Parameter Communication. ICASE, September 26, 1974, 8 pages. Submitted to IEEE Computer.
- 3. William G. Poole, Jr., Norman E. Gibbs, and Paul K. Stockmeyer: A Comparison of Several Bandwidth and Profile Reduction Algorithms. ICASE, November 15, 1974, 24 pages. Submitted to the ACM Transactions on Mathematical Software.
- 4. George J. Fix: Finite Elements and Fluid Dynamics. ICASE Report No. 75-1, February 1, 1975, 48 pages. To appear in the Proceedings of the First International Symposium on Computational Methods in Nonlinear Mechanics.
- 5. Max D. Gunzburger, C. H. Liu, and Lucio Maestrello: Simulation by Vortex Rings of the Unsteady Pressure Field Near a Jet. ICASE Report No. 75-2, February 12, 1975, 7 pages. To appear in the Proceedings of the AIAA Second Aeroacoustics Specialists Conference.
- 6. Victor R. Basili and John C. Knight: A Language Design for Vector Machines. ICASE Report No. 75-3, February 18, 1975, 14 pages. To appear in the Proceedings of the Conference on Programming Languages and Compilers for Parallel and Vector Machines.
- 7. Richard C. Raffenetti: Optimal Even-Tempered Gaussian Atomic Orbital Bases: First Row Atoms. ICASE Report No. 75-4, February 25, 1975, 12 pages. To appear in the Proceedings of the International Symposia on Quantum Theory, Part III.
- 8. David Gottlieb and Bertil Gustafsson: Generalized Du Fort-Frankel Methods for Parabolic Initial-Boundary Value Problems. ICASE Report No. 75-5, February 27, 1975, 32 pages. To be submitted to the SIAM Journal on Numerical Analysis.

# Appendix C. ICASE Seminar Program

# September 1, 1974 - February 28, 1975

September 3	Prof. Beresford Parlett, Department of Mathematics, University of California, Berkeley: "When to Stop the Lanczos Process"
September 6	Prof. Micha Wolfshtein, ICASE and Department of Aeronautical Engineering, The Technion: "Turbulence Models"
September 19	Dr. Jack Minker, Professor and Chairman of Computer Science, University of Maryland: "A Search Strategy for a Deductive Question Answering System"
September 24	Dr. Bernard C. Weinberg, Lecturer, Fluid Mechanics and Heat Transfer, University of the Negev, Israel: "Mass Transfer from Plates with Finite Sources"
September 27	Dr. John Gebhart, Director of Technology, Cadcom, Inc., Annapolis: "Mini-Computers for Computer-Aided Design"
September 30	<u>Prof. G. W. Stewart</u> , Department of Computer Science, University of Maryland: "Methods of Simultaneous Iteration for Large Eigenvalue Problems"
October 8	<u>Prof. Robert L. Ashenhurst</u> , Director, Institute for Computer Research, University of Chicago: "Hierarchical Computer Systems"
October 17	Prof. Micha Wolfshtein, ICASE and Department of Aeronautical Engineering, The Technion: "A Study of the Efficiency of Various Navier-Stokes Solvers"
October 31	Dr. Mario Schaffner, Massachusetts Institute of Technology: "A New Approach to Computers"
November 12	Prof. Leonard Brown, Department of Applied Mathematics and Computer Science, University of Virginia: "A Multi-Derivative Numerical Method for Stiff Ordinary Differential Equations"
November 18	Prof. James D. Foley, Department of Computer Science, University of North Carolina: "Graphics Systems Modeling"
November 27	Prof. Forest Baskett, Department of Computer Science, Stanford University: "A Stochastic Model of Program Paging Behavior"
December 10	Prof. Leonard A. Lopez, Department of Civil Engineering, University of Illinois: "An Approach to Automated Design"
December 13	Prof. Herbert B. Keller, Department of Applied Mathematics, California Institute of Technology: "The Box Scheme for Nonlinear Diffusion Problems"

December 17 Prof. Sam Fuller, Department of Computer Science and Electrical Engineering, Carnegie-Mellon University: "Emerging Multi-Processor Computer Structures" Dr. W. Terry Hardgrave, ICASE: "Set Processors and Large Mass January 6 Storage Devices" January 13 Prof. Vitalius Benokraitis, Department of Mathematical Sciences, Virginia Commonwealth University: "Adaptive Acceleration of SSOR for Solving Large Systems of Equations" Mr. Andrew H. Sherman, Department of Computer Science, Yale University: "Minimal Storage Techniques for Sparse Gaussian January 20 Elimination" January 27 Mr. Randolph E. Bank, Department of Applied Mathematics, Harvard University: "Fourier Direct Methods for Elliptic Boundary Value Problems" February 10 Mr. Griffith Hamlin, Jr., Department of Computer Science, University of North Carolina: "A Programming System for Use in Computer Graphics" February 13 Dr. Melvyn Ciment, Naval Surface Weapons Center: "Higher Order Compact Implicit Schemes for the Wave Equation" Prof. Roland A. Sweet, University of Colorado and National February 24-28 Center for Atmospheric Research: "Direct Methods for Poisson's Equation: An Overview;" "A Cyclic Reduction Algorithm for

Block Tridiagonal Systems of Arbitrary Dimension;" "A Package

of FORTRAN Subroutines to Solve Poisson's Equation"

The Second Langley Conference on Scientific Computing was held on October 21 and 22 in Virginia Beach, VA under the co-sponsorship of ICASE (The Institute for Computer Applications in Science and Engineering at NASA's Langley Research Center) and SIAM. 192 people registered for the meeting.

The theme of the meeting was Numerical Methods for Vector and Parallel Processors, and the first session consisted of invited tutorial/survey talks on current and future hardware. Prof. Harold Stone of the University of Massachusetts discussed processors of the Illiac IV type; Dr. John Knight of NASA's Langley Research Center described vector machines with emphasis on the CDC STAR-100 and the TI ASC; Prof. William Wulf of Carnegie-Mellon University covered multi-mini-computer complexes, illustrated by the C.m mp project at Carnegie-Mellon. These talks were very well received by the audience.

There was a total of thirty-five contributed papers. Of these, eight were concerned with Illiac IV, and thirteen with the STAR, ASC or STARAN; the remainder were directed towards general questions of parallelism without reference to particular machines. Broken down in a different direction, fourteen of the papers dealt with linear algebra algorithms, thirteen with partial differential equations and their applications, and the remaining eight with various topics ranging from quadrature to computer graphics.

One interesting aspect of the conference was the organization of a "Poster Session", a concept which has been described in the June 28, 1974 issue of Science (p. 1361). As implemented at Virginia Beach, it consisted of a session of twelve contributed papers for a duration of an hour and a half. Each speaker had a designated area in a 30' x 40' room, and a 3' x 4' cardboard poster on an easel on which to display written materials. The members of the audience moved around the room at their leisure, browsing the exhibits and spending as much (or as little) time at each paper as they wished. This allowed a good deal of personal interaction with the authors in order to clarify points, discuss related work, etc. In an informal poll of the conference attendees at the beginning of the next regular session, approximately 70% felt that such a session was a very good idea and 30% thought it a good idea; 90% indicated willingness to participate as a speaker in such a session in the future.

The conference closed with an hour and a half panel discussion on the theme: "The Impact of Parallel/Vector Computers on Numerical Analysis." The panelists were Dr. Fred Fritsch of Lawrence Livermore Laboratory, Prof. John Rice of Purdue University, Prof. Harold Stone of the University of Massachusetts, and Prof. Joseph Traub of Carnegie-Mellon University. The moderator was Dr. Robert Voigt of ICASE. Some general areas of concensus were: much has been done in the last year on how to use these processors but much more remains to be done; the existence of more and more machines should accelerate the development of algorithms; there has been relatively little involvement of the university community to date.

# I C A S E S E M I - A N N U A L R E P O R T

March 1, 1975 - August 31, 1975

INSTITUTE FOR COMPUTER APPLICATIONS

IN SCIENCE AND ENGINEERING

Operated by the

UNIVERSITIES SPACE RESEARCH ASSOCIATION

at

NASA'S LANGLEY RESEARCH CENTER

Hampton, Virginia

#### 1. Introduction

ICASE was formed in 1972 under an agreement between NASA's Langley Research Center and the Universities Space Research Association, a consortium of some fifty major universities across the country.

The primary objective of ICASE is to perform research in applied mathematics, numerical analysis, and applied computer science with particular emphasis on application areas of interest to the Langley Research Center. The mechanism of performing such research is through visiting appointments of leading university researchers in these fields, postdoctoral fellowships, and term appointments of younger scientists with no other affiliation. Such appointees, whose training is primarily in mathematics and computer science, are encouraged to work in close collaboration with NASA scientists and engineers on problems of mutual interest. It is hoped that such collaborations will contribute to the continued vitality of applied mathematics and computer science while at the same time make an immediate impact on problems of concern to NASA.

The overall research program of ICASE is directed toward the general area of scientific computing with particular emphasis on bridging the many gaps between theory and practice, and between mathematicians and computer scientists on the one hand and engineers and natural scientists on the other. The major categories of the current ICASE research program are:

- a. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR-100.
- b. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
- c. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.
- d. Computer systems and software, with particular emphasis on minicomputers, data management, and computer graphics.

The work in each of these areas will be described briefly in the next section, while other activities are discussed in Section 3.

## 2. The ICASE Research Program

#### a. Efficient Use of Vector and Parallel Computers

The major effort in this area continues to be centered around the FESS project, a cooperative effort with representatives from the Structures and Dynamics Division, Analysis and Computations Division (ACD), George Washington University (GWU), and ICASE, with the goal of producing a finite element program for STAR. Dr. James M. Ortega, Director of ICASE, has assisted Professor Ahmed Noor in directing the effort while Dr. Robert G. Voigt, Assistant Director of ICASE, and Professor William G. Poole, on leave half-time from William and Mary College from September 1, 1974 to June 1, 1975 and full time for June 1975, have been involved in developing STAR subroutines for solving the linear systems arising from finite element analysis. In collaboration with Dr. J. Lambiotte of ACD, specifications were completed for the coding of all the modules necessary. The specifications were developed using many of the ideas currently associated with the production of reliable software. It was felt that very little additional time was required to incorporate these ideas, and the resulting specifications have already proved to be a valuable form of documentation during the development period. Coding has been completed on all of the modules.

Drs. Poole and Voigt were involved in two other projects which should have impact on the FESS project. The first of these, a study of the problem of balancing I/O rate with computation rate on vector computers, was carried out in collaboration with Dr. J. Knight of ACD. The problem of solving a banded system of linear equations so large that most of the data cannot be core contained was considered. Then using instruction timings and a model of peripheral devices, a comparison of computation rate and I/O rate was made. The

analysis was parameterized so that a variety of computers, including the CDC STAR and Texas Instruments ASC, and peripheral devices could be studied. The conclusion was that for a problem of this type and existing peripheral devices, in general, the I/O rate is not satisfactory to maintain the computation rate such machines are capable of. This work was described by Dr. Voigt in an ICASE seminar, has appeared in an ICASE report, and will be presented at the 1975 ACM Conference.

The other effort of Drs. Poole and Voigt, in collaboration with Professor J. Alan George of the University of Waterloo, is centered around investigating various solution techniques for the large sparse linear systems arising in finite element analysis. In particular the approach known as substructuring (or dissection) is being investigated to determine its effectiveness on vector computers. For example, the work in progress will permit the prediction of the optimal number of substructures required to minimize the computation time for a particular vector computer. The effect of vector lengths on computation rates may make this number less than that indicated by analyses done for serial computers. It is expected that the results of this study will have an impact on the FESS project for those problems that are too large to be contained in core memory. Preliminary results of this work will be reported at the Symposium on Sparse Matrix Computation at Argonne National Laboratory in September.

Douglas Dunlop, a student assistant at ICASE, continued working with Dr. Knight on the development of a new high level programming language, SL/1, for the STAR-100; this project was started in the summer of 1974 while Dr. Knight was at ICASE and is described in the previous two semi-annual reports. A prototype compiler has now been written in PASCAL for the CDC 6600 and is producing object code for the STAR-100. Initial testing of this code on the STAR-100 itself has been carried out and the results are encouraging.

Further enhancements to both the language and the compiler - especially in the area of I/O - are planned as well as testing by a limited number of users. Professor Victor Basili of the University of Maryland is acting as consultant to this project.

Professor Harold Stone of the University of Massachusetts completed an ICASE report on sorting on the STAR-100. This work was described in the previous ICASE semi-annual report.

## b. Numerical Analysis

Dr. Alan Cline finished a two-year term appointment at ICASE and accepted a position at the University of Texas-Austin. During this reporting period he continued and completed his work on the Lanczos and conjugate gradient methods for the solution of large linear systems which was described in the last ICASE semi-annual report. An ICASE report is being written which obtains various theoretical estimates on the rate of convergence of the standard as well as minimum residual variant of the conjugate gradient method. Numerical results are presented which show the relationship of these convergence estimates to actual rates of convergence for certain test cases. Finally, a discussion is given as to when the conjugate gradient method may be competitive for banded and even dense systems. This work was presented at an ICASE seminar and will be submitted to the SIAM Journal on Numerical Analysis. In a second ICASE report in preparation, Dr. Cline analyses rounding error in the conjugate gradient method and shows that, in machine arithmetic, the convergence rate is close to the theoretical bounds derived in the first paper. He also shows that such things as loss of orthogonality are not as critical as previously believed.

An important problem with many applications is that of least squares approximation with linear inequality constraints. It has previously been known how to convert this problem into a least squares problem with non-negative

constraints - a problem for which effective algorithms are available - provided that the matrix of the least squares part of the original problem has full rank. Dr. Cline has now extended this transformation procedure so as to be able to handle matrices which are rank deficient. An ICASE report has been completed which will be submitted to the SIAM Journal on Numerical Analysis.

Dr. Cline continued work on computing the interior eigenvalues of very large sparse symmetric matrices. This work started in conjunction with Professor Gene Golub of Stanford University and Professor George Platzman of the University of Chicago on a problem of computing normal modes of oceans. Cline's current approach to this problem is to use inverse iteration after a first approximation to an interior eigenvalue has been found. Then the resulting linear system is solved by the Lanczos method. However, the Lanczos iteration is very slowly convergent when the coefficient matrix is ill-conditioned, as it necessarily is in inverse iteration. Therefore the Lanczos method is modified by, essentially, removing the eigenvalue near zero. Preliminary computations have been encouraging. Dr. Cline will describe this work in an invited talk at the Symposium on Sparse Matrix Computations at Argonne National Laboratory in September. An ICASE report is also in preparation.

Dr. Cline has extended and incorporated various codes for computing splines under tension into a comprehensive package. This will appear as an ICASE Report. He has also extended his regression package (ICASE Report, April 19, 1974) so as to be able to handle other statistical tests of importance to Donald Rummler and C. W. Stroud of the Materials Research Branch and has worked with them on its use. Finally, he collaborated with Dr. S. Park of ACD on a problem of synthesis of pictures by means of cubic splines through a small number of data points.

Dr. Jerrold Rosenbaum completed a two-year appointment at ICASE and accepted a position at Virginia Commonwealth University. The necessary and sufficient conditions for multistep-multiderivative methods for the numerical solution of ordinary differential equations to be A-stable are known, but they are difficult to apply. Dr. Rosenbaum has been developing several necessary criteria which are easy to apply and can act as an aid in the design of methods that are A-stable. The most important necessary condition is that the method must be implicit in both the solution and all derivatives that are used in the method. Other necessary conditions in terms of the maximum absolute value of rational functions along the imaginary axis have also been developed.

Dr. Poole, in collaboration with coauthors at the College of William and Mary, completed the program REDUCE for the reduction of the bandwidth or profile of sparse symmetric matrices. This program - which is the realization of an algorithm described by the authors in a previous ICASE report (November 1974) - has been issued as an ICASE report and will appear in the ACM Transactions on Mathematical Software.

Dr. Max Gunzburger, who is on a term appointment at ICASE until
September of 1976, continued his collaboration with Professor George Fix of
Carnegie-Mellon University on various boundary conditions that can be imposed
on the outflow region in viscous fluid flow problems. Work on the linearized
Burger's equation as a simple test problem was discussed in the previous
semi-annual report and was presented by Dr. Gunzburger in an ICASE seminar.
Computations are now being carried out which use their new integral condition
as a "boundary" condition in a two dimensional problem in stream-vorticity
function formulation - where such a condition arises naturally. In addition,

well-posedness of this condition for elliptic problems has been verified and error estimates for a finite element solution have been obtained, both for one space dimension. The extension of these results to two space dimensions is now being investigated.

Dr. David Gottlieb visited ICASE several times during the year while on the faculty at the Massachusetts Institute of Technology and then joined ICASE in June on a term appointment until September of 1976. In collaboration with Professor Steven Orszag of MIT, who was at ICASE for a week in July, he has been analyzing the stability of spectral methods for initial-boundary value problems for hyperbolic partial differential equations. Stability for the semi-discrete equations has now been proved for three model scalar equations and for Chebyshev polynomials as the basis functions. A unified approach is now being attempted that will handle more general equations as well as basis functions.

Dr. Gottlieb also collaborated with Dr. Eli Turkel, who spent July and August at ICASE, on a generalization of the Lax-Wendroff method for hyperbolic equations. This generalization has the same relationship to the two step Richtmyer method as the Kreiss-Oliger scheme has to the leapfrog method. Several variants based on the MacCormack method were also considered as well as extensions to parabolic problems. Extensions to two dimensions were analyzed and a proof of the stability of a Thommen-type algorithm was given. Numerical results show that the phase error can be considerably reduced from that of the second order methods and is similar to that of the Kreiss-Oliger scheme. Furthermore, the scheme can handle shocks without the addition of an artificial viscosity. This work is now complete and an ICASE report is being prepared.

Dr. Turkel also developed a composite Lax-Wendroff/Leapfrog scheme which combines the best properties of these two algorithms. For the pure

initial value problem for hyperbolic equations both stability conditions and phase errors have been analyzed. In addition it is shown that space extrapolation can be used along the boundaries although possibly with a reduced time step. For two space dimensions there are several ways of generalizing both the Lax-Wendroff and the leapfrog methods. It is proven that some of these combined Lax-Wendroff/Leapfrog schemes are unconditionally unstable while others remain stable. Numerical results confirm the improved behavior of the composite scheme. An ICASE report on this work is now being written.

Professor William Gragg joined ICASE on August 1 for a nine month appointment while on leave from the University of California - San Diego. He plans to continue first his work on secant methods for nonlinear least squares problems using a stabilized Gauss-Secant method and matrix updating techniques.

# c. Computational Research in Science and Engineering

Professor C. William Gear of the University of Illinois continued his collaboration with Dr. Roland Bowles of ACD, Dr. Rosenbaum, and Professor Leonard Brown of the University of Virginia on numerical methods for realtime simulation. The characteristics of several methods were compared using a test program that examines the response of the integrator to a step function input. The error criteria chosen were: accurate representation of the general solution near the imaginary axis, a suitably large region of absolute stability, and a step response that did not exhibit undue oscillation starting with the second order Adams Bashforth (AB2) method currently in use.

Predictor corrector methods were considered that used only one function evaluation (PEC). The conclusions are that high order predictors tend to "ring" badly, and cannot be used either by themselves or with a corrector.

However, correctors of a higher order do not have nearly as much ringing although they will have an additional delay. Thus, the AB2/AM3 combination (AM3 is the Adams Moulton 3 step method) is an acceptable combination. AB1 (Euler's method) can be used as an extrapolation formula to remove the delay without introducing serious ringing. In order to get accurate representation of the general solution near the imaginary axis, exponential fitting was studied. In this case the coefficients of the method are chosen so that it is exact for the equation y' = uy when u takes on a particular value near the imaginary axis. It was found that the coefficients of the corrector could be chosen to fit correctly a PEC combination once the coefficients of the predictor were known. Fitting a formula along the imaginary axis guarantees that the stability boundary will cross into the negative half plane at a nearby point which is undesirable. Consequently, the concept of damped exponential fit was introduced in which the response of the integrator is required to represent a very slightly damped solution at some point on the imaginary axis. BDF methods, which use past values of the solution but only current values of the derivative, were also studied. A three step AB2/BDF3 method was found to have good accuracy and response characteristics, and about the same stability region as the AB2/AM3 method. Both the AB2/AM3 and the AB2/BDF3 type methods are in the process of being tested on the Space Shuttle simulation program at Langley. Work has also begun on implementing and testing the methods on the ALTRAC simulation, which has a pilot in the loop and will be a more critical test of the integration methods than the space shuttle. It is planned that an ICASE report on these results will be prepared in the near future.

Exponential Adams methods for handling the integration of the control system and sensor parts of a real time aircraft simulation are being developed and tested. These parts of the simulation are characterized by ordinary

differential equations whose eigenvalues have large real parts (the control system) or large imaginary parts (the sensors) and the previous methods are not satisfactory. The test program has been written along similar lines as the earlier test program.

Dr. Rosenbaum has also been investigating the use of implicit methods for real time simulation.

Professor Bertil Gustafsson spent the year July 1, 1974 to July 1, 1975 at ICASE on leave from the University of Uppsala (Sweden). He completed an ICASE report with Dr. Gottlieb on the analysis of a modified version of the Navier-Stokes equations in which the total temperature is assumed to be constant and therefore the energy equation can be replaced by an algebraic relation. This problem arose in connection with work being done with the Fluid Mechanics Branch. The analysis showed that, in the inviscid case, the system is strictly hyperbolic and well-posed for the initial value problem. The Kreiss theory was then used to analyze the boundary conditions for two dimensional problems. One interesting result of this analysis was that for subsonic inflow one cannot specify the physical variables but only the characteristic variables which are certain combinations of the physical variables. This work was presented by Dr. Gottlieb in an ICASE seminar and has been accepted for publication in Studies in Applied Mathematics.

Drs. Gottlieb and Gustafsson also collaborated with members of the Fluid Mechanics Branch in analyzing their Hopscotch code. This analysis showed that the method was introducing too much dissipation and, moreover, can be used only for marching to the steady state solution since it is not consistent with the time-dependent problem. However, the results for the steady state problem are not effected by these deficiencies of the method.

Dr. Gustafsson continued his development of an ADI box-type method for calculating the flow about blunt bodies at hypersonic speeds. The

scheme is dissipative and implicit and a Newton method is used to solve the nonlinear algebraic equations. A program was written and debugged by Mr. R. Boisvert, a student assistant at ICASE, and preliminary results were obtained. Dr. Gustafsson plans to continue working on the program in Sweden.

Professor Achi Brandt of the Weizmann Institute spent the period

July 7 - August 15 at ICASE, working primarily on further developments to
his Multi-Level Adaptive Technique (MLAT) for the numerical solution of
elliptic and mixed-type partial differential equations. After a series
of three lectures on MLAT, Dr. Brandt began a collaboration with Perry

Newman and Jerry South of the Theoretical Aerodynamics Branch towards the
goal of applying MLAT to transonic flow problems. A program was written
for the small - disturbance equation as a test problem and the initial

results have been encouraging. During the coming year Dr. Brandt will be on
leave with IBM at Yorktown Heights and plans several visits to ICASE to help
in the further development of this program.

Two theoretical aspects of MLAT were also clarified during this period. First, the smoothing properties of relaxation sweeps were studied more thoroughly resulting in some general theorems for elliptic difference equations with constant co-efficients and for certain simple non-elliptic equations. Since the smoothing of residuals is the crucial step in the multi-grid process, this work gives theoretical foundation to the belief, based on computational tests, that elliptic difference equations can be solved by the multi-grid method in O(n/p + logn) operations, where n is the number of unknowns and p is the number of parallel processors. The other theoretical aspect concerns the asymptotic rate of convergence. Prof. Brandt has begun a report that will describe MLAT and collect the theoretical results that are now available.

Dr. Michael Ghil of the Courant Institute, New York University, spent the period from May 22 - August 8 at ICASE. He continued the work on the initialization problem in numerical weather prediction which was reported on in the ICASE March 1 - August 31, 1974 semi-annual report. Dr. Ghil derived a new system of equations which describe the hard-tomeasure instantaneous horizontal velocity field in terms of the more easily measured temperature field and of its first two time derivatives; this derivation was carried out for different mathematical models of large-scale atmosphere phenomena, including the one which is widely used in operational weather forecasting. The systems obtained are nonlinear and of mixed type. Type conditions were established and the connection with "wind laws" previously used in dynamical meteorology was pointed out. This work has been described in an ICASE report which will be submitted to the Journal of the Atmospheric Sciences. Dr. Ghil will pursue the analysis and numerical solution of these systems over the next academic year at the Goddard Institute for Space Studies and at the Courant Institute. During his stay at ICASE Dr. Ghil also consulted with R. E. Turner of the Analytical Studies Branch, SATD, on split-step semi-implicit numerical methods for a zonally-averaged atmospheric circulation model with applications to stratospheric pollution studies.

Prof. Micha Wolfshtein has been at ICASE on sabbatical leave since August of 1974 with the exception of a two month visit to the National Center for Atmospheric Research in Boulder, CO. In conjunction with Dr. R. Hirsh and Ms. B. Pitts of the Fluid Mechanics Branch, he completed the ICASE report - described in the previous semi-annual report - on a new ADI type method for certain nonlinear partial differential equations. The method looks very promising for the Navier-Stokes equations, in particular. This work was presented at an ICASE seminar and at the AICA

International Symposium on Computer Methods for Partial Differential Equations at Lehigh University.

Dr. Wolfshtein also completed, in conjunction with M. Atias and M. Israeli of the Technion, an ICASE report on a comparative study of the efficiency of various Navier Stokes solvers. Six methods of solution of the two dimensional vorticity-stream function equations were compared in regard to CPU time versus accuracy for an impinging jet, and a square cavity with a moving top. The results show that a Gauss Seidel solution of the central difference equations is more efficient than any other method, but it is not always sufficiently stable. Consequently, a new second order upwind scheme was recommended. This work was presented at the Second AIAA Computational Fluid Dynamics Conference in June.

In addition to the above work, Prof. Wolfshtein continued his study of turbulence modeling. Various models for the diffusion of turbulence energy in wave number space have been examined and it was decided to use an integral approximation which may be either a Heisenberg type approximation or the Kraichman direct interaction approximation. In colloboration with J. Herring of the National Center for Atmospheric Research, the quasiisotropic model for two-point correlations in physical space has been compared with the Kraichman direct interaction approximation for spectral distribution in wave number space. It was found that for axially-symmetrical, homogeneous turbulence the two models constitute Fourier transforms of one another. Finally, a study of experimental data on the "bursting" events in turbulent boundary layers revealed a deterministic chain of events within any such "burst." A numerical procedure for the calculation of this chain and its implications for drag reduction on compliant walls was suggested and a joint research proposal with Dennis Bushnell of the Fluid Mechanics Branch was submitted to the Bi-national Israeli-American Foundation.

Dr. Gunzburger has continued work on the propagation of sound in subsonic jets. Some basic physical and computational questions have been studied, including the physical correctness of linearization about mean flows, the stability of Galerkin methods for hyperbolic systems which model problems with flow, and the proper treatment of boundaries in the numerical approximation.

In collaboration with Prof. L. Ting of the Courant Institute and Dr. C. H. Liu and Mr. Lucio Maestrello of the Acoustics and Noise Reduction Division (ANRD), Dr. Gunzburger has also continued a study of the simulation of the pressure field near a jet by the shedding of vortex rings from the jet exit. Preliminary results were given in ICASE Report 75-2 (February, 1975) and recent work has centered on various refinements of the model and of the computer code. These include the inclusion of randomly shed vortices and a better modeling of the decay of the vortex rings.

Prof. Saul Abarbanel of Tel-Aviv University is spending August and September at ICASE, and is working in connection with the Advanced Entry Analysis Branch on the problem of the correct physical specification of boundary conditions on the base of a hypersonic re-entering body. In the base-attached cavity there is a slow viscous recirculating flow and the problem is how to pose the pressure boundary condition. To investigate this problem a model was chosen wherein the recirculating flow is dominated mostly by the three corner flows (at the base shoulder, at base center and at the rear stagnation point where the bubble closes). It was further assumed, on the basis of experimental and numerical evidence for supersonic cases, that the recirculating fluid is governed by the Stokes flow equation. At the rear stagnation point it was found that in order to assure symmetry about the line connecting the base and rear stagnation points the velocity towards the base must be roughly one half the characteristic shear layer

velocity. This inward velocity is a very insensitive function of the cornerangle at the rear stagnation point. A similar study near the base shoulder corner indicated how to treat numerically the pressure boundary condition along the base. This cavity study is now being generalized to the three dimensional axi-symmetric case.

Prof. Wayne Mastin is spending the period August 25, 1975 through May of 1976 on sabbatical leave from Mississippi State University. During this period he will investigate transformation techniques for mapping complex geometries into simpler ones for computational purposes. It is expected that he will work in collaboration with members of the Fluid Mechanics Branch on applying these techniques to fluid flow problems.

Dr. Richard Raffenetti, who is at ICASE on a term appointment until June of 1976, continued his collaboration with Dr. D. Phillips of the Environmental and Space Sciences Division (ESSD) and Dr. G. Pellett of the Space Applications and Technology Division on the problem of removal of chlorine from the stratosphere. Computations of the Hartree Fock energies of the complex  $NH_A$  C1 have been made varying the  $N-H_A$  and  $H_A-C1$  separation with the molecule in an overall  $C_{3v}$  geometry. A search of the potential surface reveals just a single minimum, the most stable geometry being characteristic of a molecular complex rather than a charge transfer complex as had been computed earlier by others. Further variation of the geometry in which the  $C_{3v}$  symmetry is broken is being carried out to obtain enough information about the full potential surface to do an approximate vibrational analysis. The resulting zero point vibrational energy will correct the computed vertical dissociation energy. The vibrational analysis will also provide the basis from which an estimate of the lifetime of the molecular complex may be obtained. Configuration interaction computations will also be carried

out in the near future.

Dr. Raffenetti continued his work, described in the last semi-annual report, with Dr. Phillips and Dr. E. Long of ESSD on the  $NO_3$  complex and on the dissociation of  $H_2O$ . In conjunction with Dr. Cline, he also began a study of various methods of computing eigenvalues of large sparse matrices. Among the schemes being considered are simultaneous iteration, the Lanczos method, and simultaneous coordinate relaxation.

# d. Computer Systems and Software

Prof. Stephen Sherman of the University of Houston is spending the period May 1974 to September 1976 at ICASE. Dr. Sherman is principal investigator on a supplementary NASA grant to ICASE which has allowed the acquisition of a PRIME 300 mini-computer system and associated graphics terminals. The system was installed in August 1974, and is being used to study the potentialities of a low-cost mini-computer for interactive graphics, data base management, and other possible functions. This study is being cosponsored by ACD and by the IPAD project of the Structures and Dynamics Division (SDD).

During this period, the operating system was modified to remove excess code and add extra capabilities. A message switching algorithm was implemented to allow terminal to terminal communication. The basic routines for file transfer which were used in the high level communication system VENUS - discussed in the previous semi-annual report - were improved.

Dr. Sherman collaborated with Mr. David Loendorf, a Civil Service employee of the Army who is assigned to SDD, on the development of a prototype data base management system (BETKA). This has been implemented on the PRIME 300 and is now being used by various people although improvements to the system are still being made. Douglas Dunlop contributed to this project by rewriting the high-level routines using LANGPAK so as to make the language more

flexible.

Dr. Sherman also worked with Dr. Richard Brice of George Washington University on constructing a software probe for the PRIME. This probe instruments various key sections of the system and records such things as paging information, scheduling information, and requests for system service on a magnetic tape for later analysis. Drs. Brice and Sherman are using this probe to study the general question of buffer management in data base systems and, in particular, the interaction of the following four factors: paging algorithms, buffer handling algorithms, real memory size, and buffer size as a function of the total  $I/\emptyset$  in the system, i.e. the paging  $I/\emptyset$  plus normal  $I/\emptyset$  to the disks. The data base system BETKA is being used as a representative system that is heavily dependent on I/Ø for performance. A series of experiments on the PRIME are almost complete and preliminary analysis indicates that the most important factors are memory size and buffer size. Moreover, it appears that an increase in buffer size does not necessarily yield worse performance. Further analysis of the experiments is continuing.

Dr. W. Terry Hardgrave finished his term appointment at ICASE and accepted a position at the University of Maryland. He completed a number of projects discussed in the previous semi-annual report. An ICASE report on set processing in a network environment was prepared and submitted to the Communications of the ACM. This report, together with another on the use of the Set-Theoretic Data System developed by STIS, Inc. constituted the final report for the supplemental NASA grant NSG 1068. The MP3/SGOL macro-processor was also completed. It is installed on the Prime mini-computer and is being installed on the Kronos system at Langley. It will be maintained by Douglas Dunlop.

Dr. Hardgrave also completed the first stage in the development of an information system based on set theory; a prototype system has been implemented on the Prime mini-computer. This system currently accepts character strings, integers, and real numbers as atoms (i.e. data types) and allows sets, n-tuples, relations, and arbitrarily deep nestings of any of these, as structures. Matrices will be added in the near future. It has been used so far to query some test data bases and will be used by other people at ICASE as an experimental system. The system was described in an ICASE seminar and Dr. Hardgrave is currently preparing two reports on its implementation and use. He also collaborated with Dr. Poole on preliminary investigations of possible uses of the system in scientific computation.

Dr. Poole, and Mr. Boisvert completed an interactive graphics package - which is implemented on the Prime as well as the CDC 6000's - for automatic node renumbering of finite element matrices. This work will appear as an ICASE report and is to be presented at the Conference on Applications of Computer Graphics in Engineering.

Prof. Richard Phillips of the University of Michigan spent the period July 1 - August 31 at ICASE working in conjunction with David Loendorf and other members of the IPAD Development Section to evaluate the data management requirements of an integrated aircraft design program. An existing preliminary design program, GASP, was used as the environment for this study after being converted to run on the PRIME 300. Various data management functions - such as data base building, retrieval, and modifications - were integrated into the program and the data base itself was built by GASP using the BETKA system described above. Each design in the data base consists of a design node to which is attached 14 data nodes representing geometry, engine data, etc. In order to facilitate communication between

the designer and the data base a symbol table was produced which relates the name of a design variable, such as gross weight, range, etc., to a position in a data node. Next, a query language and retrieval program was developed that permits casual scanning of the data base, as well as identification of a design by a combination of detailed design attributes. A design can be depicted graphically in the form of an annotated three-view once the user has identified designs of interest.

Future directions for this research involve extension of the query capability, paying special attention to graphical techniques, full integration of data management facilities into GASP, and the addition of another level of preliminary design capability, such as finite element analysis of aircraft components. Prof. Phillips plans to carry on this work at the University of Michigan during the coming year.

All of the above work on the mini-computer project has benefited substantially from the programming support of Ms. M. Castano, Mr. R. Murphy, and Mr. A. Woodruff, student assistants at ICASE.

Prof. T. L. Boardman of the University of Michigan was at ICASE from May through August 1975 and worked on the development of a microcomputer-based graphics system for the Tektronix 4014 terminal. This system will permit the 4014 to operate in both store and refresh modes by maintaining a copy of the segmented screen image on a floppy disk. In addition, the microcomputer will perform two and three dimensional rotation, translation, and scaling on image segments. A general purpose microcomputer, having a base cycle time of 300 nanoseconds, was built to provide these functions for the 4014 around the Intel 3000-series microprocessor chips. This processor is capable of providing arithmetic and logical functions, memory access, and basic timing and control to as many as eight logic units.

The 4014 graphics system requires only four such units allowing the micro-processor to be timeshared by other computer-hardware projects. The system is almost complete and will be finished by Dr. Boardman during the next several weeks.

Dr. Boardman and Mr. Loendorf also made an initial study of the feasibility of implementing certain parts of finite element calculations by means of specially tailored microprocessors. This work will continue throughout the next year.

Prof. Susan Gerhart of Duke University spent the period May 5 to August 22 at ICASE studying various aspects of software engineering. She worked closely with Mr. G. E. Migneault of the Flight Instrumentation Division on several questions arising in the development of fault-tole-rant computing systems and, in particular, ways to identify and classify programming errors according to their prevention, detection, and recovery characteristics. She also worked on related questions with Dr. Terry Straeter of ACD.

In addition to this work on NASA problems, Dr. Gerhart completed an ICASE report that develops the view that there are two distinct theories - a mathematical theory of programs and an explanatory theory of programming - which are evolving from, and which subsume, the subjects of correctness proofs of programs and structured programming. Three specific topics are used to illustrate the differences and similarities in the theories: the goto statement, the problem of program specifications and the nature and use of abstractions. This work will appear in the Infotech State of the Art Reports.

Dr. Gerhart also investigated alternative ways of explaining and structuring a program for evaluating B-splines. This program was proposed by Prof. John Rice of Purdue University as one to which it is difficult to

apply the structured programming approach and obtain a program which is both understandable and efficient. A first draft of a possible ICASE report has been completed which uses the above program as an example in the context of a more general exposition of how the analysis and structuring of programs should proceed.

## 3. Other ICASE Activities

Preparations are complete for a conference on Applications of Computer Graphics in Engineering to be sponsored by NASA-Langley and cosponsored by ICASE. The meeting will be held at Langley Research Center on October 1 and 2, 1975, and will include about a dozen invited lectures as well as contributed papers. David Loendorf is Coordinator for the conference and Drs. Ortega and Voigt are serving on the Conference Committee.

Planning for the Third ICASE Conference on Scientific Computing is also complete. The meeting will be held on April 1 and 2, 1976 in Williamsburg, Virginia on the theme of Computer Science and Scientific Computing. There will be invited lectures by a number of computer scientists on the state of certain areas such as mini and microcomputers, reliability, graphics, data handling, future architecture, languages, and symbolic computation which are relevant to scientific computing. Complementary to these talks will be invited lectures in a number of applications areas.

Several ICASE members have been involved in teaching activities.

Dr. Gunzburger taught a second year graduate course on partial differential equations at George Washington University during the spring semester, while Dr. Wolfshtein offered an advanced topics course on turbulent flow at Old Dominion University. Dr. Boardman, Mr. Loendorf, and Dr. Phillips gave a one week intensive Short Course on Computer Graphics at ICASE which was attended by over fifty people. Dr. Ortega continued as coadvisor (with Prof. Bruce Chartres) of the Ph.D. dissertation of J. Lambiotte of ACD at the University of Virginia, which was completed in May.

In the professional societies, Dr. Cline continued as coeditor of the Algorithms Department of the Communications of the Association of Computing Machinery (ACM) and as Associate Editor of the ACM Transactions on Mathematical Software. Prof. Gragg is continuing on the Editorial Board of Numerische Mathematik and as an Editor of the SIAM Journal on Numerical Analysis. Dr. Poole is serving as Technical Program Chairman for the SIGCSE Symposium to be held in Williamsburg in July of 1976. Dr. Ortega continued as a member of the Program Committee of SIAM and as a member of a panel sponsored by the National Science Foundation to report on computer science research. This is a two to three year study whose goal is to document the current state of research in all areas of computer science and computer engineering and to make projections of future directions and efforts. The steering committee of the overall study is being chaired by Prof. B. W. Arden, a member of the ICASE Scientific Council.

Almost all ICASE members consulted with various NASA personnel in addition to the collaborative research described in the previous section.

#### Appendix A. ICASE Staff

March 1 - August 31, 1975

## I. Administrative

James M. Ortega, Director Ph.D., Mathematics, Stanford University, 1962 Numerical Analysis

Robert G. Voigt, Assistant Director Ph.D., Mathematics, University of Maryland, 1969 Numerical Analysis

Margaret H. Mann, Secretary

Linda T. Johnson, Secretary (Part-time)

Barbara K. Porter, Secretary (Part-time)

## II. Scientific Council

Bruce W. Arden, Professor and Chairman of Computer Sciences and Electrical Engineering, Princeton University.

James C. Browne, Professor of Computer Science and of Physics at the University of Texas at Austin.

Samuel D. Conte, Professor and Chairman of Computer Science, Purdue University.

Eugene Isaacson, Professor of Mathematics, Courant Institute, New York University.

# III. Term Appointments

Alan K. Cline - Ph.D., Mathematics, University of Michigan, 1970. Computational Linear Algebra and Approximation Theory. At ICASE September 1973 through August 1975.

David Gottlieb - Ph.D., Numerical Analysis, Tel Aviv University, 1972. Numerical Solution of Partial Differential Equations. Joined ICASE June 1975. Current appointment runs to September 1976.

Max D. Gunzburger - Ph.D., Mathematics, New York University, 1969. Fluid Dynamics and Numerical Solution of Partial Differential Equations. Joined ICASE September 1973. Current appointment runs to September 1976.

# III. Term Appointments (continued)

W. Terry Hardgrave - Ph.D., Computer Science, University of Texas at Austin, 1972. Data Management and Operating Systems. At ICASE January 1974 through August 1975.

Richard C. Raffenetti - Ph.D., Physical Chemistry, Iowa State University, 1971. Computational Quantum Chemistry. Joined ICASE in March 1974. Current appointment runs to June 1976.

Jerrold S. Rosenbaum - Sc.D., Applied Mathematics, Columbia University, 1971. Numerical Solution of Ordinary Differential Equations. At ICASE August 1973 through August 1975.

# IV. Visiting Scientists and Consultants

Saul S. Abarbanel - Ph.D., Theoretical Aerodynamics, Massachusetts Institute of Technology, 1959. Professor of Applied Mathematics and Vice-Rector, Tel-Aviv University. Numerical Solution of Partial Differential Equations. At ICASE August 4 to October 3, 1975.

Victor B. Basili - Ph.D., Computer Science, University of Texas at Austin, 1970. Associate Professor of Computer Science, University of Maryland. Programming Languages and Compiler Construction. At ICASE May 14-15, June 4-5, and August 18-19, 1975.

Thomas L. Boardman - Ph.D., Mechanical Engineering, Purdue University, 1973.
Assistant Professor of Industrial and Operations Engineering, University of Michigan.
Computer Graphics and Computer-aided Design. At ICASE May 5 to August 29, 1975.

Achi Brandt - Ph.D., Applied Mathematics, New York University, 1967. Professor of Applied Mathematics, Weizmann Institute of Science (Israel). Numerical Solution of Partial Differential Equations. At ICASE July 7 to August 15, 1975.

Leonard Brown - Ph.D., Computer Science, University of Illinois, 1974. Assistant Professor of Computer Science, University of Virginia. Numerical Solution of Ordinary Differential Equations. At ICASE May 12 to July 4, 1975.

George J. Fix - Ph.D., Mathematics, Harvard University, 1968. Professor and Chairman of Mathematics at Carnegie-Mellon University. Numerical Methods for Partial Differential Equations. At ICASE May 27 - 30 and July 15 - 18, 1975.

- C. William Gear Ph.D., Mathematics, University of Illinois, 1960. Professor of Computer Science and Applied Mathematics, University of Illinois. Numerical Solution of Ordinary Differential Equations. At ICASE March 5 7 and May 12 through June 20, 1975.
- J. Alan George Ph.D., Computer Science, Stanford University, 1971. Associate Professor of Computer Science, University of Waterloo. Numerical Linear Algebra and Finite Element Methods. At ICASE May 14 16 and August 26 28, 1975.

Susan L. Gerhart - Ph.D., Computer Science, Carnegie-Mellon University, 1972. Assistant Professor of Computer Science, Duke University. Program Correctness. At ICASE May 5 to August 22, 1975.

## IV. Visiting Scientists and Consultants (continued)

Michael Ghil - Ph.D., Applied Mathematics, New York University, 1975. Research Associate at NASA Goddard Institute for Space Studies and Adjunct Assistant Professor at Courant Institute. Numerical Solution of Partial Differential Equations and the Equations of Dynamic Meteorology. At ICASE May 26 to August 8, 1975.

Gene H. Golub - Ph.D., Mathematics, University of Illinois, 1959. Professor of Computer Science at Stanford University. Numerical Solution of Large-scale Matrix Problems. At ICASE April 21 - 22, 1975.

William B. Gragg, Jr. - Ph.D., Mathematics, University of California at Los Angeles, 1964. Professor of Mathematics at University of California, San Diego. Numerical Analysis. At ICASE August 1, 1975 through May 1976.

Bertil Gustafsson - Ph.D., Computer Science, University of Uppsala (Sweden), 1968. Acting Professor of Computer Science, University of Uppsala. Numerical Solution of Partial Differential Equations. At ICASE July 1, 1974 to June 30, 1975.

C. Wayne Mastin - Ph.D., Mathematics, Texas Christian University, 1969. Assistant Professor of Mathematics at Mississippi State University. Conformal Mapping. At ICASE August 25, 1975 to May 1976.

Steven A. Orszag - Ph.D., Physics, Princeton University, 1966. Professor of Applied Mathematics, Massachusetts Institute of Technology, Computational Fluid Dynamics. At ICASE July 15 - 19, 1975.

Richard L. Phillips - Ph.D., Aerospace Engineering, University of Michigan, 1964. Professor of Aerospace Engineering, and Computer, Information and Control Engineering University of Michigan. Computer Graphics and Data Base Management. At ICASE July 7 to August 29, 1975.

William G. Poole, Jr. - Ph.D., Computer Science, University of California at Berkeley, 1970. Assistant Professor of Mathematics at the College of William and Mary. Computational Linear Algebra. At ICASE half-time from September 1, 1974 to June 1, 1975, and full-time the month of June 1975.

Stephen W. Sherman - Ph.D., Computer Science, University of Texas at Austin, 1972. Assistant Professor of Computer Science at the University of Houston. Operating Systems and Mini-computers. At ICASE May 6, 1974 through August 1976.

Eli Turkel - Ph.D., Applied Mathematics, New York University, 1970. NSF Fellow at Courant Institute, New York University. Numerical Solution of Partial Differential Equations. At ICASE July 1 to September 1, 1975.

Micha Wolfshtein - Ph.D., Mechanical Engineering, University of London, 1968. Senior Lecturer, Aeronautical Engineering, The Technion, Israel. Computational Fluid Dynamics. At ICASE August 18, 1974 to June 13, 1975 and August 18 to October 3, 1975.

# v. Affiliated Langley Member

David D. Loendorf - M.S., Structural Engineering, Old Dominion University, 1970. M.S., Computer, Information, and Control Engineering, University of Michigan, 1974. Application of Computer Graphics to Structural Engineering. Assigned to the Structures and Dynamics Division of Langley Research Center by the Army Air Mobility Research and Development Laboratory.

# VI. Student Programming Assistants

Ronald F. Boisvert - Graduate Student at William and Mary College. At ICASE August 1974 through August 1975.

Marjorie E. Castano - Undergraduate at Christopher Newport College. At ICASE June 1974 through August 1975.

Douglas D. Dunlop - Undergraduate at William and Mary College. At ICASE since January 1975.

Ronald C. Murphy - Undergraduate at Christopher Newport College. At ICASE since June, 1974.

Arthur L. Woodruff - Graduate student at William and Mary College. At ICASE June 1975 through August 1975.

#### Appendix B. ICASE Reports

#### March 1, 1975 - August 31, 1975

- 1. Knight, John C.; Poole, William G., Jr.; Voigt, Robert G.: System Balance Analysis for Vector Computers. ICASE Report No. 75-6, March 21, 1975, 25 pages. To appear in the Proceedings of the 1975 ACM National Conference.
- 2. Hardgrave, W. Terry: Set Processing in a Network Environment. ICASE Report No. 75-7, March 31, 1975, 43 pages. Submitted to the Communications of the ACM.
- 3. Hardgrave, W. Terry: Accessing Technical Data Bases Using STDS: A Collection of Scenarios. ICASE Report No. 75-8, April 16, 1975, 84 pages.
- 4. Crane, H. L., Jr.; Gibbs, Norman E.; Poole, William G., Jr.; Stockmeyer, Paul K.: Matrix Bandwidth and Profile Reduction. ICASE Report No. 75-9, April 14, 1975, 19 pages. Submitted to ACM Transactions on Mathematical Software.
- 5. Hirsh, Richard S.; Pitts, Barbara H.; Wolfshtein, Micha: Second-Order Non-Iterative ADI Solution of Non-Linear Partial Differential Equations. ICASE Report No. 75-10, May 12, 1975, 7 pages. Published in the Proceedings of the AICA International Symposium on Computer Methods for Partial Differential Equations.
- 6. Atias, M.; Wolfshtein, Micha; Israeli, M.: A Study of the Efficiency of Various Navier-Stokes Solvers. ICASE Report No. 75-11, May 12, 1975, 10 pages. Published in the Proceedings of the Second AIAA Conference on Computational Fluid Dynamics.
- 7. Gottlieb, David; Gustafsson, Bertil: On the Navier-Stokes Equations with Constant Total Temperature. ICASE Report No. 75-12, June 2, 1975, 33 pages. Accepted for publication in Studies in Applied Mathematics.
- 8. Stone, Harold S.: Sorting on STAR. ICASE Report No. 75-13, June 5, 1975, 32 pages. Submitted to the IEEE Transactions on Software Engineering.
- 9. Cline, Alan K.: The Transformation of a Quadratic Programming Problem into Solvable Form. ICASE Report No. 75-14, August 11, 1975, 14 pages. Submitted to the SIAM Journal on Numerical Analysis.
- 10. Gerhart, Susan L.: On the Relationship Between Structured Programming and Correctness Proofs. ICASE Report No. 75-15, August 13, 1975, 26 pages. To appear in the Infotech State of the Art Reports.
- 11. Ghil, Michael: Initialization by Compatible Balancing. ICASE Report No. 75-16, August 22, 1975, 38 pages. Submitted to the Journal of the Atmospheric Sciences.

# Appendix C. ICASE Seminar Program

# March 1, 1975 - August 31, 1975

March 10	Mr. George W. Cox, Computer Science Department, Purdue University: "Portability and Adaptability in Operating System Design."
March 14	Mr. Wayne D. Dominick, Department of Computer Science, Northwestern University: "Graphically-Enhanced Data Base Management System Design."
March 18	Mr. John W. Lewis, Computer Science Department, Yale University: "CURVED: Spline Curve Editing."
March 21	Prof. Jack Lipovski, Department of Electrical Engineering and Computer Information Sciences, University of Florida: "A Non-Numeric Architecture: CASSM."
March 24	Prof. M. R. Stonebraker, Department of Electrical Engineering and Computer Sciences and the Electronics Research Laboratory, University of California, Berkeley: "INGRES - A Relational Data Base System."
March 28	Prof. C. Wayne Mastin, Department of Mathematics, Mississippi State University: "The Construction of Curvilinear Meshes for Multiply Connected Regions by Conformal Mappings."
April 3	Dr. Robert G. Voigt, ICASE: "System Balance Analysis for Vector Computers."
April 3	Dr. Stephen W. Sherman, ICASE: "The PRIME Mini-computer."
April 14	Prof. Bertil Gustafsson, ICASE and the University of Uppsala: "Generalized Du Fort-Frankel Methods for Parabolic Initial-Boundary-Value Problems."
April 16	Prof. Jim Douglas, Jr., Department of Mathematics, University of Chicago: "Various Methods of Imposing Dirichlet and Neumann Boundary Conditions for Elliptic and Parabolic Finite Element Methods."
April 24	Prof. Peter J. Denning, Computer Science Department, Purdue University: "Dynamic Behavior of Multi-programming."
May 2	<pre>Prof. Richard Flower, Department of Electrical Engineering, University of Illinois: "Topics in the Complexity of Data Bases."</pre>
May 7	Prof. Susan L. Gerhart, ICASE and Computer Science Department, Duke University: "Toward a Mathematical Theory of Program Correctness."

May 12 Prof. Thomas L. Boardman, ICASE and Department of Industrial and Operations Engineering, University of Michigan: placement for the CRT Graphics Terminal: The Plasma Panel." May 30 Dr. Michael Ghil, ICASE and Courant Institute of Mathematical Sciences: "A Nonlinear Parabolic Equation with Applications to Climate Theory." June 3 Prof. Micha Wolfshtein, ICASE and the Technion: "Second-Order Non-Iterative ADI Solution of Nonlinear Partial Differential Equations." June 5 Dr. H. Robert Howie, Ampex Corporation: "The TBM Mass Storage System." June 6 Prof. Olaf Widlund, Courant Institute of Mathematical Sciences: "The Capacitance Matrix Method for the Helmholz Equation." Dr. Alan K. Cline, ICASE: "A Survey of Methods for the June 11 Determination of Eigenvalues of Large Matrices." June 23 Prof. Henryk Wozniakowski, Computer Science Department. Carnegie-Mellon University: "Numerical Stability of the Chebyshev Method for the Solution of Large Linear Systems." July 2 Prof. Eli Turkel, ICASE and Courant Institute of Mathematical Sciences: "Fourth Order Methods for Hyperbolic Equations." July 7 Prof. Richard L. Phillips. ICASE and Department of Aerospace Engineering and the Computer, Information, and Control Program, University of Michigan: "A Special Purpose Programming Language for Data Analysis." Prof. Achi E. Brandt, ICASE and Department of Applied Mathe-July 14, 16, matics, Weizmann Institute of Science: "The Multi-Level and 18 Adaptive Technique (MLAT) and Applications to Transonic Flow Problems." July 15 Dr. Max D. Gunzburger, ICASE: "Downstream Boundary Conditions for Viscous Flow Problems." July 17 Prof. Steven A. Orszag, Department of Mathematics, Massachusetts Institute of Technology: "Progress in Numerical Simulation of Turbulence." Dr. David Gottlieb, ICASE: "On the Navier-Stokes Equations July 22 with Constant Total Temperature." Dr. Alvin Bayliss, Courant Institute of Mathematical Sciences: July 25 "Almost Periodic Solutions to Difference Equations." Prof. Dennis Severance, Department of Operations Research, Cornell University: "A Practitioner's Guide to Addressing July 28 Algorithms."

- Dr. Michael Ghil, ICASE and Courant Institute of Mathematical August 4 Sciences: "Initialization by Compatible Balancing." August 7 Prof. Richard Bucy, Departments of Aerospace Engineering and Mathematics, University of Southern California: "Discrete -Time Nonlinear Estimation." August 11 Dr. Alan K. Cline, ICASE: "Convergence of the Lanczos and Conjugate Gradient Algorithms for the Solution of Large Sparse Systems of Linear Equations." August 13 Prof. Moshe Goldberg, Mathematics Department, University of California, Los Angeles: "A Stable Approximation for Hyperbolic Systems with Moving Internal Boundary Condition." <u>Dr. W. Terry Hardgrave</u>, ICASE: "A Scientific Information System (SIS) Based on a Set Processor." August 18 <u>Prof. Richard L. Phillips</u>, ICASE and Department of Aerospace Engineering and the Computer, Information, and Control Program, August 27 University of Michigan: "Production and Display of a Data Base Generated by a General Aviation Synthesis Program."
- August 29 Prof. Robin McLeod, Department of Computer Science, University of Manitoba: "Basis Functions for Curved Elements in the Finite Element Method."